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Computer Program for Calculating and Fitting Thermodynamic Functions

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National Aeronautics and
Space Administration
Office of Management
Scientific and Technical
Information Program

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Summary

A computer program is described which (1) calculates thermodynamic functions (heat capacity, enthalpy, entropy, and Gibbs energy) for several optional forms of the partition function, (2) fits these functions to empirical equations by means of a least-squares fit, and (3) calculates, as a function of temperature, heats of formation and equilibrium constants.

The program provides several methods for calculating ideal gas properties. For monatomic gases, three methods are given which differ in the technique used for truncating the partition function. For diatomic and polyatomic molecules, five methods are given which differ in the corrections to the rigid-rotator harmonic-oscillator approximation. A method for estimating thermodynamic functions for some species is also given.

Introduction

The computer program PAC1 (Properties and Coefficients), documented in reference 1, was initially made available to outside organizations in 1967. Since that time, PAC1 has been continuously revised, updated, and extended. Inasmuch as the program continues to be widely requested and used, this report is being published to provide documentation for the current version, referred to as PAC91.

The two principal purposes for initially preparing PAC1 are still valid today, namely, (1) to provide a means for generating theoretical thermodynamic functions from molecular constant data and (2) to provide a means of fitting these functions to empirical equations by using a least-squares fit. The coefficients obtained from the fit may then be used to generate a library of thermodynamic data in a uniform and easy-to-use format for use in other computer codes. Several large compilations of selected or calculated thermodynamic data currently exist. (See refs. 2 to 4 for some examples of early compilations and refs. 5 to 9 for some examples of more recent compilations.) Nevertheless, in spite of these compilations, there is a continuing need for additional calculations due to (1) discovery of new species, (2) revision of existing molecular constant data and structural parameters, (3) need for data at temperatures other than those already published, (4) availability of new or revised heats of formation, dissociation, or transition, and (5) revision of fundamental constants or atomic weights. Calculations may also be needed to compare the results of assuming

various possible forms of the partition function. In addition, as mentioned previously, there is often a preference for thermodynamic data in functional rather than tabular form.

In order to carry out these needs, the PAC91 program has been prepared to perform any combination of the following: (1) calculate thermodynamic functions (heat capacity, enthalpy, entropy, and Gibbs energy) for any set of 1 to 202 temperatures, (2) obtain a least-squares fit of the first three of these functions (either individually, two at a time, or all three simultaneously) for up to eight temperature intervals, and (3) calculate, as a function of temperature, heats of formation and equilibrium constants from assigned reference elements. The number 202 for temperatures is somewhat arbitrary but was selected to accommodate a schedule of temperatures from 100 to 20 000 K at every 100 K, $T = 298.15$ K, and one additional temperature, if desired, such as $T = 273.16$ K.

The thermodynamic functions for ideal gases may be calculated from molecular constant data using one of several partition function variations provided by the program. For monatomic gases, (1) one of three partition function cutoff techniques may be selected and (2) unobserved but predicted electronic energy levels may be included by the program. For diatomic and polyatomic gases, (1) one of five partition functions may be selected which differ in the correction factors for nonrigid rotation, anharmonicity, and vibration-rotation interactions and (2) excited electronic states may be included.

Several new capabilities that were added to the program since the last publication include (1) the estimation of thermodynamic properties by a group additivity method, (2) the ability to calculate properties for species with internal rotors, and (3) a method for extrapolating data to high temperatures.

For the purpose of additional processing, (1) known thermodynamic functions for solids, liquids, or gases may be read in directly or (2) thermodynamic functions may be calculated from heat capacity equations.

Because of the variety of options provided and the resulting variety of input data required, an objective was to provide for a relatively simple procedure for reading input data. This was accomplished by means of a uniform input format.

At the time reference 1 was written (1967) input was read in by means of punched cards. While punched cards are no longer used, 80-column records are still retained for input.

The program and the equations used are described in detail. Examples of input and output are given for a variety of species.

Calculation of Ideal Gas Thermodynamic Functions

For gaseous species, the thermodynamic functions may be calculated from spectroscopic constants. A general discussion of methods of calculation is given in references such as 1 and 8. Many of the equations will be repeated here for convenience. The properties are expressed as functions of the internal partition function Q ; that is,

$$\frac{C_p^\circ}{R} = T^2 \frac{d^2(\ln Q)}{dT^2} + 2T \frac{d(\ln Q)}{dT} + \frac{5}{2} \quad (1)$$

$$\frac{H_T^\circ - H_0^\circ}{RT} = T \frac{d(\ln Q)}{dT} + \frac{5}{2} \quad (2)$$

$$\frac{S_T^\circ}{R} = T \frac{d(\ln Q)}{dT} + \ln Q + \frac{3}{2} \ln M + \frac{5}{2} \ln T + S_c \quad (3)$$

$$-\frac{G_T^\circ - H_0^\circ}{RT} = \frac{S_T^\circ}{R} - \frac{H_T^\circ - H_0^\circ}{RT} = \ln Q + \frac{3}{2} \ln M + \frac{5}{2} \ln T + S_c - \frac{5}{2} \quad (4)$$

where

$$S_c = \frac{5}{2} + \ln \left[\left(\frac{2\pi m_e k T_1}{h^2} \right)^{3/2} \frac{k T_1}{p_o} \right] \quad (5)$$

S_c is the Sackur-Tetrode constant. ($T_1 = 1$ K. Other symbols are defined in appendix A.) When $p_o = 100\,000$ Pa (1 bar), $S_c = -1.151693$. When $p_o = 101\,325$ Pa (1 atm), $S_c = -1.164856$. Thus, values of S_T°/R in units of bars will be higher than corresponding values in units of atm by 0.013163. The values for S_c and other fundamental constants are obtained from reference 10. The values of these constants are contained in BLOCK DATA of the program and are given in the section BLOCK DATA.

The internal partition function Q in equations (1) to (4) is given by

$$Q = \sum_{m=1}^L Q^m \quad (6)$$

where Q^m is the internal partition function for the m^{th} electronic state and L is the number of electronic states.

Internal Partition Functions for Monatomic Gases

For monatomic molecules, internal energy consists of electronic energy only. Equation (6) then becomes

$$Q = \sum_{m=1}^L Q_e^m = \sum_{m=1}^L (2J_m + 1) e^{-\epsilon_m/kT} = \sum_{m=1}^L g_m e^{-\epsilon_m/kT} \quad (7)$$

where Q_e^m , J_m , ϵ_m , and g_m are the electronic energy partition function, total angular momentum quantum number, electronic excitation energy, and statistical weight, respectively, for the m^{th} electronic state.

Cutoff methods.—An infinite number of bound states exist below the ionization limit for a hypothetical isolated atom ($L = \infty$ in eq. (7)). Inasmuch as the partition function diverges and approaches infinity as $L \rightarrow \infty$, the summation must be cut off. Reviews of various cutoff methods are given in a number of references such as 1, 8, 11, and 12. The following review essentially repeats that given in reference 1.

The cutoff methods may be considered to be of the following types:

- (1) No dependence on temperature or pressure
- (2) Dependence on temperature only
- (3) Dependence on temperature and pressure (or density) and possibly degree of ionization

In the first of the three types, the summation may include various numbers of levels. For example, only the ground state is used in the Saha equation (see ref. 13) and only valence states are included in reference 8. The summation of equation (7) may be over a fixed and usually arbitrary number of levels (as, e.g., in ref. 14) or equation (7) may be summed through all observed levels (as in ref. 15, e.g.).

The second cutoff type is temperature dependent. The ionization potential is reduced by a quantity referred to as the ionization potential lowering, which in this case is a function of temperature only. The partition function is then permitted to include only those levels below the lowered ionization potential. In reference 16 it was suggested that the ionization potential be lowered by an amount equal to the temperature function kT . This suggested method was used in reference 4. Other temperature functions are summarized in reference 11.

The first two cutoff types are distinguished by the fact that they permit the partition function and related thermodynamic properties to be calculated as functions of temperature only. For the third type, it is not possible to calculate the partition function by specifying temperature only. One cutoff technique of this type relates the highest permitted principal quantum number n to the number of particles per unit volume (number density) such as suggested by Bethe (see discussion in ref. 11). Another technique uses the ionization potential lowering procedure previously described, but in this case the quantity by which the potential is lowered is a function of electron and ionized particle number densities. Several such quantities are summarized in reference 11.

This last technique involves mixtures of species and therefore precludes, for all practical purposes, the possibility of generating tables for individual species as a function of

temperature only. This is due to the fact that the cutoff criterion needed to calculate the partition function depends on mixture composition, while the calculation of mixture composition depends on the partition function. Thus, an iterative procedure is required where the partition function at a specified temperature may be changing from one iteration to the next. Consequently, since PAC91 calculates thermodynamic properties only for pure species, just the first two cutoff types are considered in this report.

Inclusion of predicted levels.—In addition to the divergence problem, there is the problem of whether to include observed energy levels only or to also include levels for predicted terms which, so far, have not been observed. From atomic theory, as presented in texts such as reference 17, predicted terms can be derived. Some of these terms are given in tables 10 and 11 in reference 17; in tables 5 to 20 in reference 18; and in reference 19. An examination of the tabulated observed terms in references 18 and 19 shows that many predicted terms are missing, especially for the higher quantum numbers.

It has been shown that various series of levels can be represented by formulas such as the Rydberg or the Rydberg-Ritz formulas (e.g., ref. 20). The constants in these formulas can be determined from known levels and used to extrapolate for the unobserved levels. However, the number of observed levels differ from species to species and, therefore, some judgment must be exercised in obtaining these constants. An alternate, but considerably simpler, technique for filling in unobserved levels, which gives essentially the same results for the partition function for many species as does the use of the Rydberg-Ritz equations, is included in the program. This alternate technique will now be described.

When the statistical weights g_i corresponding to predicted terms were examined, it was determined that for many chemical elements the sum of the statistical weights can be expressed by the following simple function of the principal quantum number n (except for the ground state n of most species):

$$\sum g_i = \sum (2J_i + 1) = bn^2 \quad (8)$$

Equation (8) applies only to terms arising from excitation of the emission electron and does not account for other possible terms. A table in reference 1 contains, for the first 20 chemical elements, (1) the derived constants b to be used in equation (8) to obtain $\sum g_i$ for any n above the ground state and (2) $\sum g_i$ values for the ground state. In reference 12, this table was extended to include all the first 86 elements except for the lanthanide series (elements 58 through 71). Table 5 from reference 12 (p. 28) appears in this report as table I. The total quantum number above the ground state is given as a function of n in equation (8). However, in reference 12 it was recommended that, for some elements, the total quantum number above the ground state should be taken as a constant

value (called c^*) for all values of n . Values of c^* are given in table I for elements 21 through 28, 39 through 46, 57, and 72 through 78.

The usefulness of equation (8) arises from the fact that the inclusion of an unobserved level generally makes considerably more difference in the partition function than does the error in the estimated energy for this level. Therefore, an option is provided in the PAC91 program to determine for each n the difference in statistical weight sums between the observed levels which have been read in as input and that given by equation (8). The program then adds this difference to the g_i of the highest observed level for the corresponding n .

This method of filling in predicted, but unobserved, levels by means of equation (8) was used to calculate the thermodynamic functions of the atomic species in reference 4.

Internal Partition Function for Diatomic and Polyatomic Molecules

Partition function.—For diatomic and polyatomic molecules, Q^m in equation (6) involves vibrational and rotational as well as electronic energy. In this report the following factored form is used to calculate Q^m :

$$Q^m = Q_e^m Q_v^m Q_R^m Q_\rho^m Q_\theta^m Q_W^m Q_c^m$$

or

$$\ln Q^m = \ln Q_e^m + \ln Q_v^m + \ln Q_R^m + \ln Q_\rho^m \\ + \ln Q_\theta^m + \ln Q_W^m + \ln Q_c^m \quad (9)$$

A recent review of formula details for these individual contributions to Q is given in reference 8. Some earlier references are as follows. The quantities Q_e^m , Q_v^m , and Q_R^m are the electronic, harmonic-oscillator, and classical-rotation contributions to the partition function, respectively, as given in standard texts (see refs. 21 to 24). The remaining quantities in equation (9) are the following correction factors: rotational stretching (centrifugal distortion) Q_ρ^m (refs. 24 to 26), low-temperature rigid rotation Q_θ^m (refs. 24 and 27), Fermi resonance Q_W^m (ref. 28), and both anharmonicity and vibration-rotation interaction Q_c^m (refs. 29 to 31).

The program provides five methods of calculating the partition function which vary in the inclusion of, and formulas for, the correction terms ($\ln Q_\rho^m$, $\ln Q_\theta^m$, $\ln Q_W^m$, and $\ln Q_c^m$). This provision is made so that the results of the various methods may be compared.

Table II contains detailed formulas for all the $\ln Q^m$ terms and their derivatives except those for $\ln Q_e^m$ which are given in table III. The derivatives of $\ln Q_c^m$ are not given directly as are the derivatives in table II. It was found to be considerably more convenient to express the derivatives of $\ln Q_c^m$ by means of general formulas than to obtain the derivatives directly. These general formulas are given in a footnote to table III.

Internal rotations.—A number of species, such as propylene oxide or hydrogen peroxide, have internal rotation. Energy levels for internal rotation may be calculated from potential functions, usually of the form

$$V = \frac{1}{2} \sum V_n (1 - \cos n\phi) \quad (10)$$

where V is the potential, V_n an n -fold barrier, n an integer from 1 to 6, and ϕ the phase angle. These energy levels may then be used to calculate the internal rotation contribution to the thermodynamic functions.

A computer program for calculating the energy levels and thermodynamic functions for the equation (10) potential was written by J. Laane and Associates based on the analysis in reference 32. This program was incorporated into PAC91 with necessary modifications. In addition, an option was added to calculate the contribution of a free rotor.

The subroutines which are involved in the hindered rotation calculation are INTROT, IROTOR, HMAT, EIGEN, and PRINT. A brief description of these routines is given in the section **Main Routines and Subroutines**.

Group Additivity Method

Several methods are available for estimating thermodynamic properties when molecular constant data for calculating partition functions are not available (e.g., see refs. 33 to 39). One of these methods is the group additivity method. S.W. Benson and coworkers have presented extensive tables of group properties for use with this method (refs. 35 and 36). These group properties permit estimating the heat of formation and entropy at 298.15 K and heat capacities from 300 to 1000 or 1500 K (depending on the group). In reference 37 Stein presents heat capacity properties to 3000 K for 18 groups pertaining to hydrocarbons.

Specialized techniques exist for obtaining estimates from group properties which may give more accuracy than that of Benson's method (e.g., refs. 38 and 39). However, Benson's method is accepted for PAC91 because of its relative simplicity, good accuracy, and application to a wide variety of species.

Empirical Equations For Thermodynamic Functions

Empirical equations for thermodynamic functions are often used for convenience. In dimensionless form, equations for heat capacity are usually of the following type:

$$\frac{C_p^o}{R} = \sum_{i=1}^r a_i T^{q_i} \quad (11)$$

where the exponent q_i may be zero or either a positive or negative whole or fractional number.

Enthalpy and entropy are related thermodynamically to C_p^o/R as follows:

$$\frac{H_T^o}{RT} = \frac{b_1}{T} + \int \frac{C_p^o}{RT} dT \quad (12)$$

$$\frac{S_T^o}{R} = b_2 + \int \left(\frac{C_p^o}{RT} \right) dT \quad (13)$$

where b_1 and b_2 are integration constants.

In equation (12) all terms are divided by T in order to make the equation dimensionless. The program uses equations (11) to (13) in two ways: (1) in generating the coefficients a_i and b_j from a set of thermodynamic data using the least-squares technique given in reference 40 or (2) conversely in generating the thermodynamic data from the empirical equations. Some details of the least-squares method are given in the section **Least-squares fit**.

Assigned Enthalpy Values

For some applications (see ref. 41) it is convenient to combine sensible enthalpy and energies of chemical and physical changes into one numerical value. An arbitrary base may be adopted for assigning absolute values to the enthalpy of the various substances, inasmuch as only differences in enthalpy are measurable. For example, the arbitrary base selected in reference 4 was a value of zero at 298.15 K ($H_{298.15}^o = 0$) for a selected set of elements. This base was also selected for PAC91. It makes the assigned value, $H_{298.15}^o$, of any substance equal to its heat of formation at 298.15 K from this set of selected elements.

Assigned Reference Elements

The designation of an element in a particular phase to be a reference element is needed in order that values of heats of formation $\Delta_f H_T^o$ and equilibrium constants $\log_{10} K$ be unambiguously related to specific reactions. Reference 42 gives thermodynamic functions, phases, transition temperatures, and heats of transition for the following 50 elements plus deuterium and election gas: Ag, Al, Ar, B, Ba, Be, Br₂, C, Ca, Cd, Cl₂, Co, Cr, Cs, Cu, D₂, e⁻, F₂, Fe, Ge, H₂, He, Hg, I₂, K, Kr, Li, Mg, Mn, Mo, N₂, Na, Nb, Ne, Ni, O₂, P, Pb, Rb, S, Si, Sn, Sr, Ta, Th, Ti, U, V, W, Xe, Zn, and Zr. The enthalpy and free energy values from reference 42 have been stored on a file (referred to herein as the EF data file) for the purpose of $\Delta_f H_T^o$ and $\log_{10} K$ calculations.

Heats of Formation and Equilibrium Constants

In the program described in this report, heats of formation and $\log_{10}K$ for a species are calculated as functions of temperature for the formation of the species from the elements in their assigned reference state. The following is an example of how these properties are calculated for CO(g) at 1000 K:

$$\Delta_f H_{1000}^o = (H_{1000}^o)_{CO(g)} - (H_{1000}^o)_{C(graphite)} - \frac{1}{2} (H_{1000}^o)_{O_2(g)} \quad (14)$$

$$\Delta_f G_{1000}^o = (G_{1000}^o)_{CO(g)} - (G_{1000}^o)_{C(graphite)} - \frac{1}{2} (G_{1000}^o)_{O_2(g)} \quad (15)$$

By definition,

$$\log_{10}K = \frac{-\Delta_f G_T^o}{2.3025851 RT} \quad (16)$$

Computer Program

The computer program PAC91 was written in ANSI standard Fortran 77. PAC91 should work on any system with sufficient storage. There are about 5500 lines in the source code which uses about 300 kilobytes of memory. The compiled program takes about 390 kilobytes.

Some input and output files are stored in the standard I/O units 5 and 6, respectively. Other I/O units are used in conjunction with least-squares coefficients, EF data sets, and group additivity data (see section "Saved Output" in appendix C). These nonstandard I/O units are as follows:

I/O unit	Contents or function
10	Least-squares coefficients
11	Formatted EF data
13	Unformatted EF data
14	Scratch unit for formatted EF data
17	Scratch unit for unformatted EF data
19	Group additivity data

No OPEN statements for the I/O units were included in the source program.

Availability to Other Organizations

The PAC91 program can be obtained for a fee from COSMIC (Computer Software Management Information

Center) at the following address:

COSMIC
382 East Broad Street
Athens, GA 30602
Tel: (404) 542-3265
FAX: (404) 542-4807

The program will generally be sent out on a diskette which contains the following four files:

File number	Contents
1	PAC91 source program
2	EF data sets for reference elements
3	Least-squares coefficients for additivity groups
4	Input data sets for examples

The preparation of files 2 and 3 is discussed in the section "Saved output" in appendix C. File 4 contains the input for the eight examples given in appendix D which can serve as test cases for checking out the program. Files 2, 3, and 4 require approximately 160, 24, and 10.2 kilobytes, respectively.

Input Data Codes

The input for a particular species is a set of 80-column records. There are many alphanumeric code words in these records. These code words use capital letters and numbers and have a maximum length of six characters. They either (1) indicate an option; (2) identify a record; or (3) describe the information that follows it.

These code words will be used throughout the report. The input code words in columns 1 to 6 will be referred to as record IDs. Elsewhere on the record, they will be referred to as labels. An index of code words is given in table XI which may be helpful in locating definitions, discussions, and examples. A complete discussion of input format is given in appendix B.

Options

The program provides a choice of several methods for calculating the thermodynamic functions C_p^o , $H_T^o - H_0^o$, $H_T^o - H_{298.15}^o$, S_T^o , $-(G_T^o - H_0^o)$, and $-(G_T^o - H_{298.15}^o)$. For ideal gases, these functions may be obtained from one of several assumed forms of the partition function, from empirical equations, or, for some hydrocarbons, from the group additivity method. For solids and liquids, the thermodynamic functions may be calculated only from empirical equations. In addition, thermodynamic functions for any phase of a species may be read in directly for additional processing.

The program also has two other capabilities which are optional: (1) least-squares fitting of the thermodynamic functions to empirical equations (eqs. (11) to (13)) and (2) calculating heats of formation and $\log_{10}K$ values for the same temperature range as the functions.

The following is a discussion of these optional features.

Partition functions—monatomic gases.—The partition function for monatomic gases is given by equation (7). The program permits three optional ways of terminating the number of energy levels L to be included in calculating this partition function. These three options, indicated by their input code names, are: (1) ALLN—inclusion of all electronic levels in the input data, (2) FIXEDN—inclusion of all levels through a specified principal quantum number n , and (3) TEMPER—inclusion of all energy levels that are less than or equal to the ionization potential lowered by an amount kT (see section **Cutoff methods**).

With any of these three cutoff options, an additional option (FILL) is provided to include predicted but unobserved levels automatically (see discussion in the section **Inclusion of predicted levels**). All of these options are labels on the METHOD record (see table VI).

Partition functions—diatomic and polyatomic gases.—For diatomic and polyatomic gases, the program provides for a selection of five methods of calculating the partition function. These methods vary in the inclusion of, and formulas for, the correction terms ($\ln Q_\rho$, $\ln Q_\theta$, $\ln Q_w$, and $\ln Q_c$) in equation (9). The formulas for the $\ln Q$ terms included in each of the five methods are given in tables II and III. If certain spectroscopic constants are not available as input, the program automatically excludes those $\ln Q$ terms involving them. The methods (with their METHOD record labels given in parentheses) are as follows:

(1) Rigid-Rotator Harmonic-Oscillator (RRHO) approximation—This method excludes all the correction terms in equation (9) (i.e., $\ln Q_\rho$, $\ln Q_\theta$, $\ln Q_w$, and $\ln Q_c$).

(2) Modified Pennington and Kobe (PANDK) method—The formulas given in table III for $\ln Q_c$ are similar to those given in reference 29. The method in this report is equivalent to the one described in reference 4 except for the formula for $\ln Q_\theta$ (formula 6 in table II). All correction terms in equation (9) are included with the exception of the Fermi resonance $\ln Q_w$ as indicated in table II.

(3) Joint Army Navy Air Force (JANAF) method—This method is described and used in reference 6. For diatomic molecules, it is the same as the PANDK method except for the definitions of a_1 and X_{11} which are used in formulas 9 and 12, respectively, in table III. For polyatomic molecules, the JANAF method is the same as the RRHO method.

(4) Nonrigid-Rotator Anharmonic-Oscillator 1 (NRRAO1)—In addition to the $\ln Q_\theta$ and $\ln Q_\rho$ terms, all the $\ln Q_c$ terms given in references 30 and 31 were included which do not contain a $(c_2/T)^2$ or $(c_2/T)^3$ factor.

(5) Nonrigid-Rotator Anharmonic-Oscillator 2 (NRRAO2)—This method includes the same $\ln Q_c$ terms as NRRAO1 with the addition of $\ln Q_c$ terms from references 30 and 31 which contain $(c_2/T)^2$ factors.

METHOD record labels are summarized in table VI.

Internal rotation contributions.—As described in the section **Internal rotations**, PAC91 includes the capability of calculating

the contributions of internal rotation, free or hindered. The contribution of each internal rotor replaces the contribution of a fundamental frequency. Thus the total number of fundamental frequencies (including degeneracies) plus the number of internal rotors remains $3N-6$, where N is the number of atoms in the molecule.

Estimation by group additivity method.—As mentioned previously, PAC91 provides an option for estimating thermodynamic properties by a group additivity method. At present, thermodynamic properties for just 34 groups have been prepared for use with PAC91 (see section **Input**). These group properties permit estimating properties for some but not all hydrocarbons (e.g., groups for cyclic and fused hydrocarbons are not included). The group properties are in the form of least-squares coefficients with C_p° represented as a fourth-order polynomial. The additivity method requires identifying the various groups comprising the species. This is discussed further in the sections **Input** and **Data records for ADD method** in appendix B and in example 2 in appendix D).

Thermodynamic functions from empirical equations.—The routine for calculating thermodynamic functions from the empirical equations (eqs. (11) to (13)) has the following features:

(1) The value of r (number of coefficients a_i) may be any number from 1 to 8.

(2) The temperature exponents q_i may be zero or any positive or negative whole or fractional number.

(3) Any number of sets of a_i and q_i may be read in for various temperature intervals for a particular species.

(4) The integration constants b_1 and b_2 may be read in or calculated by the program from the enthalpy and entropy values, respectively, for a specific temperature.

(5) When a phase transition occurs, the integration constants b_1 and b_2 for the second phase may be read in or calculated by the program from either the enthalpy or entropy of transition.

(6) There is an option to write the heat capacity coefficients and the two integration constants for each temperature interval on I/O unit 10.

Least-squares fit.—The least-squares routine fits the thermodynamic functions C_p°/R , H_f°/RT , and S_f°/R to equations (11), (12), and (13) either individually, any two simultaneously, or all three simultaneously (the default option). The selection of the appropriate labels for fitting any one function or any two simultaneously is discussed in the section **LSTSQS record(s)** in appendix B. The least-squares fit has the following additional features:

(1) The value of r (number of coefficients a_i) may be any number from 1 to 8. (In PAC1, r was 1 to 10.)

(2) The temperature exponents q_i may be zero or any positive or negative whole or fractional number.

(3) An option is provided to permit the data to be divided into any number of specified intervals from 1 to 8. The purpose in providing for several intervals is to increase the accuracy of the fit. (In PAC1, the number of intervals was 1 to 9.)

(4) The equations for each temperature interval are usually

constrained at an endpoint to fit either the original data or the values obtained from fitting an adjacent interval. However, there is an option to remove the constraint by use of the label NOCNS. The purpose of these constraints is to give equal values of the functions at the common point and thus avoid discontinuities between consecutive intervals. Also, only one temperature may be specified in the input for which the fitted equations reproduce the original values. (If no temperature is specified, the program assigns 298.15 K. In PAC1 the default assigned temperature was 1000 K.)

(5) For two or more phases, if an enthalpy of transition (labeled DELTAH) or an entropy of transition (labeled DELTAS) is given, the original data as well as the least-squares fitted data will be constrained so that $T\Delta_r S_T^o = \Delta_r H_T^o$.

(6) For each temperature interval, the coefficients a_i for heat capacity plus the two integration constants will be written on I/O unit 10. (In PAC1, these data were punched on binary cards.)

(7) If the temperature exponents q_i (EXP labels on the LSTSQS records) are not specified, PAC91 defaults to the following form of equation (11):

$$\frac{C_p^o}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (17)$$

and corresponding forms for H_T^o/RT and S_T^o/R (see table VIII).

(8) The equations for C_p^o/R may be the same or different for each temperature interval.

(9) At least as many values of C_p^o (or C_p^o/R) are required as the number of exponents in equation (11) or equation (17). If fewer C_p^o (or C_p^o/R) values are given in the input than the number of exponents requested, PAC91 automatically reduces the number of exponents to the number of C_p^o or C_p^o/R values.

It should be noted that the present format for the least-squares coefficients differs from that of PAC1. Details of the present format are given in table VIII.

Extrapolation by Wilhoit's method.—Occasionally data are given in the literature to only relatively low temperatures (say to 1000 or 1500 K) but data may be needed to higher temperatures for some applications (such as shock tube data analysis). As has been pointed out (see ref. 5), extrapolation of thermodynamic data with the functional form described in the previous section may give bad results. An example is the extrapolation of data for iso-octane which are given in reference 7 to 1500 K. The least-squares coefficients which are generated from these data give an extrapolated value at 3000 K of $C_p^o/R = -3331$. This impossible situation can be avoided by obtaining extrapolated values from a method for fitting data presented by Wilhoit (ref. 43). Wilhoit gives the following equation for C_p^o :

$$C_p^o = C_p^o(0) + [C_p^o(\infty) - C_p^o(0)] y^2 \left[1 + (y-1) \sum_{i=0}^n a_i y^i \right] \quad (18)$$

where $y = T/(T+S)$ (y varying from 0 to 1), S a scaling factor, $C_p^o(0)$ the low temperature limit for C_p^o , $C_p^o(\infty)$ the high temperature limit for C_p^o , and a_i the least-squares coefficients. $C_p^o(0)$ includes only rotational and translational contributions ($C_p^o(0) = 3.5R$ for linear and $4R$ for nonlinear species) while $C_p^o(\infty)$ also includes the vibrational contributions. The total contributions result in $C_p^o(\infty) = (3N-1.5)R$ for linear and $(3N-2)R$ for nonlinear species, where N is the number of atoms in the molecule.

A computer program for this method with $n = 3$ in equation (18) is given in appendix B of reference 5. This program was somewhat modified and incorporated into PAC91 as subroutines WILHOI and WCALC. While the original Wilhoit method is presented in reference 43 as a method of fitting data rather than extrapolating data, PAC91 uses these subroutines only for the purpose of extrapolation. The general procedure involved in PAC91 in using these subroutines is

(1) The original input data are fitted to Wilhoit's functional form and the Wilhoit coefficients are generated.

(2) These coefficients are then used to extrapolate the thermodynamic data to various specified temperatures.

(3) The original data and the extrapolated data are then refit to the PAC91 functional form.

For the example of iso-octane mentioned previously, the use of the Wilhoit fit for extrapolation gives a reasonable value of $C_p^o/R = 75.299$ at 3000 K. (The classical value is $C_p^o(\infty)/R = 76$.) Additional examples using Wilhoit extrapolation are given for examples 2 and 3 in appendix D.

In addition to the usual input data, the use of the Wilhoit method for extrapolation requires a WILH label on a METHOD record. The program also requires knowledge with this method of whether the species is linear or nonlinear. Unless specified otherwise, the program assumes the species is nonlinear. For linear species, the label LINE is required.

Heat of formation and $\log_{10}K$ values.—The program provides an option for calculating, as a function of temperature, heats of formation and $\log_{10}K$ values of a species formed from its reference elements (see sections **Assigned Reference Elements and Heats of Formation and Equilibrium Constants**). These values for a particular species can be calculated if the necessary enthalpy and free energy data for the reference elements (referred to as EF data) are available. Therefore, the assigned reference elements are processed first. For these reference elements there is an option to save the enthalpy and free energy data in two ways: (1) in an unformatted form on I/O unit 13 replacing any data for the element already in the library and (2) in a formatted form appending the data on I/O unit 11. (See appendix C for additional information on the contents of EF data saved on

I/O unit 11.) The data on I/O unit 13 are ready for immediate use. For backup purposes, the data on I/O unit 11 may be transferred to and included in a file containing EF data in formatted and readable form for all reference elements which have already been processed. These files replace the set of punched binary EF data cards of reference 1.

The data on I/O unit 13 are saved for use with other species being processed during the same computer run as well as for later computer runs. The data in the formatted EF data file discussed previously may be read in as part of the input and, if so, are automatically put on I/O unit 13. The newly read-in data replace data already on I/O unit 13 for any matching elements.

If there is a temperature in the data for a particular species which is not contained in the EF data for the required reference elements, the reference elements data are interpolated using three-point Lagrangian interpolation.

Output tables.—There are many options for listed output tables indicated on an OUTPUT record. The tables vary in the following ways: in whether they are original data or calculated from least-squares coefficients; in energy units (dimensionless, joules, or calories); and in whether the functions are given to many figures or are rounded and include columns for $\Delta_f H_T^\circ$ and $\log_{10} K$.

Input

Input data sets for any number of species may be combined into one file. The data in each set are read, processed, and cleared before the next set is read. A set of data for a diatomic gas, for example, would contain the chemical formula; the output options; the method of calculation, such as PANDK; molecular data such as ω_e , $\omega_e x_e$, B_e , and α_e ; desired options such as a least-squares fit or a special temperature schedule; and, finally, the record ID FINISH to indicate the end of the set of data.

In addition to these input data sets, data contained in two general files are required for certain applications. The first of these two files contains enthalpy and free energy data (EF data) for reference elements which are used to calculate equilibrium constants $\log_{10} K$ and heats of formation $\Delta_f H_T^\circ$ (see section **Heat of formation and $\log_{10} K$ values**). An example of the contents of the EF data file for the element Mg is given in appendix D, example 6. The second general file contains thermodynamic data (in the form of least-squares coefficients) for various groups that are used to estimate properties of species (see section **Group Additivity Method**). These coefficients for 34 groups are given in table X and have the same format as that described in table VIII but these use a fourth-order polynomial for C_p° .

The references from which most of the data were taken to generate these coefficients are given in table IX. In addition, table IX gives the labels used in PAC91 for these groups, Benson's notation (ref. 36), the group structure, and the atoms contained in the group. Of the 34 groups given, thermo-

dynamic data for 18 were taken from reference 36 and 12 from reference 37. Thermodynamic properties for the remaining 4 groups were calculated by the PAC91 program using data from the following references:

Species		References	
Formula	Name	$\Delta_f H_{298.15}^\circ$	Spectroscopic constants
C ₂ H ₂	Acetylene	7	8
C ₂ H	Ethynyl radical	44	45
C ₂ H ₄	Ethylene	7	46,47
C ₂ H ₃	Vinyl radical	44	8
C ₂ H ₃	Stabilized vinyl radical	^a 44,48	^b 8
C ₆ H ₆	Benzene	7	49
C ₆ H ₅	Phenyl radical	7	49

^a $\Delta_f H_{298.15}^\circ$ is taken to be the same as that for the vinyl radical plus an estimated resonance stabilization energy of 8 kcal/mole taken from reference 48.

^bAssumed to be the same as for the vinyl radical.

Uniform format.—Many types of input are used in PAC91. To facilitate the preparation of this input, a uniform format was devised for the original version of this program (ref. 1) for most input data. This format is retained for the present program as well. While in the original version, input was read in from 80 column punched cards, in the present program input is in the form of 80 column records. Details of the uniform format are given in appendix B.

Contents of individual records.—A brief description of the contents of the individual records is given in table IV. (Detailed descriptions are given in appendix B.) The right-hand column indicates which records are optional. The word in columns 1 to 6 on all records except the formula record will be referred to as the record ID. Words in other columns will generally be referred to as labels. While the record ID may contain up to six characters the PAC91 program will use only the first four characters of the code to identify the record. The code is intended to be a mnemonic device. Thus, for example, the LSTSQS record contains information for the least-squares fit of the thermodynamic data. Since the program uses only the first four characters, the word LSTS is required for this record, while characters in columns 5 and 6 are optional.

As shown in table IV, the record ID does one or more of the following:

- (1) Indicates what information is in the record (e.g., NAME, REFN, OUTPUT, TEMP, LSTSQS, or CTEM).
- (2) Identifies the data on the records which follow it (e.g., METHOD and EFDA).
- (3) Calls for some intermediate output (i.e., LISTEF).
- (4) Indicates the end of a set of data (i.e., FINISH).

General Flow of Program

- (1) Each record (except for the EF data) is read and listed. The flow is directed according to the record ID.

(2) The input data (including options) are cleared at the beginning of the program and after each FINISH record ID.

(3) There may be any number of sets of data—each having any combination of options and each ending with a FINISH code.

(4) The records NAME, formula, LSTSQS, OUTPUT, DATE, and REFNCE should come ahead of the METHOD record but their order is immaterial.

(5) Any record ID ahead of the METHOD record ID which is not recognized by PAC91 will be assumed to be a chemical formula record.

(6) From the chemical formula, the following items are determined by the program:

- (a) molecular weight
- (b) phase of the species
- (c) number of atoms (i.e., whether species is monatomic, diatomic, or polyatomic)

(7) The H_0° value may be calculated from an assigned enthalpy value at any temperature or a heat of formation (see chemical formula record in appendix B and table V). (The H_0° value is used in calculating $\Delta_f H_T^\circ$ and $\log_{10} K$ and the integration constant b_1 (eq. (12)).

(8) The temperature schedule (TEMP record), if not the standard 100(100)6000 K, must be read before each METHOD record giving the calculation method. However, it should be noted that TEMP records are not used with method READIN inasmuch as temperatures for the READIN method are given on the data records.

(9) The data records must follow the METHOD record.

(10) Thermodynamic functions are calculated immediately after PAC91 reads a record ID different from the one it was reading in the data records.

(11) After the FINISH code is read, a check is made for the LSQS and LOGK options from the OUTPUT record. Also, tables of thermodynamic functions are listed (from original data and, if the CTAB label is on the OUTPUT record, from least-squares coefficients).

(12) With an EFTAPE label on an OUTPUT record for a reference element, the EF data for that element will be written on I/O units 11 and 13. The data on I/O unit 13 will be available for use with any succeeding calculations.

(13) Any number of sets of METHOD record and corresponding data records may be read for a set of input data. This is useful for species with more than one phase in the temperature range of interest. For example, the thermodynamic functions for the solid may be read in directly while the liquid data may be obtained from empirical equations. The data for both phases will appear in the same listed tables of the thermodynamic properties.

(14) Contributions of excited electronic states may be included in the calculation of the thermodynamic functions for diatomic and polyatomic gases. There may be any number of states, each having its own set of molecular constants. This is accomplished by grouping the data records for each state together with a code number in columns 79 and 80. The values

of Q^m , $T dQ^m/dT$, and $T^2 d^2Q^m/dT^2$ are calculated after the data records for each state are read. These values are summed as they are calculated.

Output

Most of the output are tables of thermodynamic data. These data may be *original* data calculated by PAC91 according to one of the methods specified by a METHOD record or the data may be calculated from least-squares coefficients generated by PAC91 with the LSQS option. Original data tables have the word ORIGINAL on the first line of the table and on the last line of each page. Tables with data from least-squares coefficients have the word COEFFICIENTS on the first line of the table and on the last line of each page.

Other possible types of output include input data, the least-squares errors table, EF data, and intermediate output. A brief description of output data is given in this section. Additional details are given in appendix C.

Input data.—The contents of all input records in the uniform format are always listed in the output. Some additional information calculated by PAC91 such as molecular weight and Wilhoit parameters are interspersed with the record images.

Tables of thermodynamic properties.—There may be ten possible tables of functions printed for the temperature schedules. The tables vary according to the labels on the OUTPUT records. Five are for *original* data. With a CTAB label, a corresponding five possibilities are for thermodynamic functions calculated from the least-squares coefficients. With the MFIG label, three of the five possible tables are given to many figures (usually from 6 or 7 to 10 or 11). With the LOGK label, the remaining two tables are rounded to the same number of figures as in the JANAF tables (ref. 6) and also may contain values of $\Delta_f H_T^\circ$ and $\log_{10} K$. The three many-figured tables and the two rounded tables vary in the energy units which must be specified with label options. The JOULES label is required for energy units in joules and the CAL label for energy units in calories. Only the many-figured tables have an option for dimensionless units (label DMLESS). The temperature schedule for the *original* data is either the default schedule, temperatures read in with data, or a schedule set by the TEMP records. The coefficients data will have the same schedule unless a special schedule is given with CTEM records.

Table of least-squares errors.—These tables are listed with the LSQS option. They provide information concerning the accuracy of the fit. The word "error" in the output refers to the difference between the original and fitted data. In addition to listing the least-squares coefficients for each temperature interval, the following information is listed: (1) the thermodynamic functions (both the original and those obtained from the least-squares fit for each temperature, (2) the errors between the original and the fitted data for each temperature, and (3) average, maximum, and least-squares errors and relative errors for C_p°/R , $(H_T^\circ - H_0^\circ)/RT$, S_T°/R , and $-(G_T^\circ - H_0^\circ)/RT$.

Intermediate output.—With an INTERM label on the OUTPUT record, additional intermediate data are listed as detailed in appendix C. These intermediate data are often useful for debugging purposes.

EF data.—EF data for a reference element contain the enthalpy and Gibbs energy data for that reference element. These data are required for $\log_{10}K$ and $\Delta_f H_f^\circ$ calculations for compounds containing that element. See sections **Listed Output** and **Saved Output** in appendix C for additional discussion of EF data.

Examples

Eight sample problems were selected to illustrate a number of the methods and options of PAC91. The input data files, listed output and some discussion of these examples are given in appendix D.

Main Routine and Subroutines

The previous program (PAC1) consists of a main routine and 17 subroutines. The present program (PAC91) consists of a main routine, 24 subroutines, and BLOCK DATA. One function, KD, was dropped from the previous program and eight new subroutines and BLOCK DATA were added. Of these eight new subroutines, five are for internal rotation (EIGEN, HMAT, INTROT, IROTOR, and PRINT); two are for extrapolation by the Wilhoit method (WCALC and WILHOI); and one is for the group additivity method (GROUP). The remaining 16 subroutines from PAC1 were extensively revised to accommodate more modern computers.

A short description of each subroutine follows.

ATOM.—This routine calculates thermodynamic functions for monatomic gases.

The routine calls INPUT to read all data records plus the next record. The J_i or g_i values (eq. (7)), which are read with an alphanumeric format, are changed to floating point numbers and stored.

Energy levels are sorted in order of increasing energy values. The number of levels included in the calculations is determined by the cutoff method (ALLN, FIXEDN, or TEMPER) given on the METHOD record. Predicted but unobserved levels will be included with the FILL option.

DELH.—This routine has several functions. It calculates the H_0° value from information given on the formula card (either heat of formation at 298.15 K (HF298), heat of formation at any temperature ($\Delta_f H_f^\circ$) and the corresponding temperature T , or an assigned enthalpy H_f° and the corresponding temperature T). If a LSQS label has been included on the OUTPUT record, subroutine LEAST is called to perform a least-squares fit. Subroutine PUNCH is called to write least-squares coefficients on I/O units 6 and 10. The coefficients may also have been read in with method COEF if a TCOEF label is included on the data records.

Subroutine DELH is called from the main program after the FINISH card has been read. However, it will also be called

from RECO for phase transition points. In this latter case, any processing (the H_0° calculation, the least-squares fit, or the writing of coefficients) will be for the species phase coming ahead of the transition point in the input. For example, for a species with input data for the solid followed by the liquid, DELH will process the solid when it has been called from RECO. The liquid will be processed when DELH is called from the main program.

DERIV.—This subroutine calculates the first and second derivatives of the logarithm of Q_c^m (the anharmonicity and vibration-rotation interaction contribution to the total partition function Q^m). It uses the special method given in footnote e of table III. The routine is called from a number of places in LINK1. The values of the variables in the call vector of DERIV are calculated in LINK1.

EFTAPE and entry EFLIST.—Subroutine EFTAPE and entry EFLIST are concerned with preparing, reading, and writing the enthalpy and free energy data records of reference elements (EF data). These EF data are used in conjunction with the option of calculating tables of $\log_{10}K$ and $\Delta_f H_f^\circ$ for any species. Subroutine EFTAPE is called under two circumstances: (1) if an EFTAPE label is included on an OUTPUT record of a reference element and (2) if an EFDA record is read. Entry EFLIST is called when a LISTEF record is read.

In the first case of subroutine EFTAPE being called (by an EFTAPE label on the OUTPUT record), the formatted EF data set for the reference element being processed is written on I/O units 6 and 11 and the unformatted data set is written on I/O unit 13.

An EF data set for the reference element currently being processed may already exist on I/O unit 13 from a previous run or from being read in from a special file (see section **Saved output**). In this event, the EF data set for the current run replaces the existing EF data set for this reference element on I/O unit 13. Otherwise, the current EF data set is written at the end of all other EF data sets on I/O unit 13.

In the second case (EFDA record is read), subroutine EFTAPE is called to read data created in the first case and previously written on I/O unit 11. These data are usually backup data or data that come with the program. The subroutine merges the data with the unformatted form of the data on I/O unit 13.

Entry EFLIST writes the contents of I/O unit 13 into I/O unit 6 in order to obtain a legible listing of the EF data for all reference elements currently in the I/O unit 13 file.

EIGEN.—This is one of the five subroutines associated with the calculation of the contribution of internal rotation to thermodynamic functions. It is called by HMAT and solves for the eigenvalues of the Hamiltonian matrix which are then used to obtain the energy levels of the rotor(s).

GROUP.—Subroutine GROUP is called from the Main Program when the label ADD is included on the METHOD record. Subroutine GROUP locates and adds together the contributions of various groups specified in the input. The group contributions are in the form of least-squares coefficients

(see table X) and, when added together, produce the least-squares coefficients for the desired species. Occasionally, for a special configuration such as gauche, a constant correction is required for H_f^o/R . For this case, the correction may be included in the input with the label HRCO.

HMAT.—This is one of the five subroutines associated with the calculation of the contribution of internal rotation to thermodynamic functions. It calculates the elements HINT (I,J) for a Hamiltonian matrix. It is called by IROTOR. HMAT, in turn, calls EIGEN to solve the matrix for the energy levels of the rotor.

IDENT.—This routine analyzes the chemical formula on either the formula record or the EFDA record. It separates and stores each chemical symbol and corresponding number of atoms in the chemical formula. The chemical symbols are matched with the SYMBOL array stored from BLOCK DATA. Corresponding indexes are stored. When analyzing a chemical formula from a formula record the molecular weight is calculated.

INPUT.—This routine is called from the main program. It reads and lists all standard input from I/O unit 5 except the thermodynamic data following the EFDA record and unformatted data. I/O unit 14 is used as a scratch unit for reading in data.

INTROT.—This is one of the five subroutines involved with internal rotation. It calculates the contribution of the internal rotor(s) to the partition function and its first and second derivatives. It uses the energy levels which are generated in subroutines HMAT and EIGEN. It is called from LINK1.

IROTOR.—This is one of the five subroutines involved with internal rotation. It is called from POLY if the label INTROT appears in the input data set. IROTOR calls INPUT to obtain the necessary input for internal rotation calculations (hindered or free). The potential function is then calculated and stored for optional printout (see subroutine PRINT). IROTOR then calls HMAT to set up a Hamiltonian matrix which is then solved in EIGEN to obtain the energy levels for the rotor. For each rotor present, IROTOR then calculates the relative value of the energy levels of the rotor above the lowest energy for that rotor. A maximum of four unique rotors is permitted.

LEAST.—This routine is called from DELH only if the LSQS label was included on the OUTPUT record. It calculates the least-squares coefficients and lists certain information comparing original thermodynamic functions with those calculated from the coefficients. See **Tables of least-squares errors and Least-squares coefficients** in appendix C.

LINK1.—This routine calculates the partition function for diatomic and polyatomic gases. The formulas given in tables II and III are evaluated according to the method specified.

The routine is called from subroutine POLY. LINK1 in turn calls two subroutines, DERIV to calculate the derivatives of the partition function and QSUM to keep a running total of the various contributions to the partition function.

LOGK.—This routine is called from the main program only if a LOGK label has been included on the OUTPUT record. It calculates $\Delta_f H_f^o/RT$, $\Delta_f H_f^o$, $-\Delta_f G_f^o/RT$, and $\log_{10} K$ for the formation of the species from the assigned reference elements.

The required enthalpy and free-energy data for these reference elements have been previously stored in the file on I/O unit 13 by the EFTAPE subroutine.

The LOGK routine lists the two tables of rounded properties as detailed in appendix C. If any required data for the reference elements of the species being processed are not on I/O unit 13, the appropriate columns in these two tables are left blank.

PAGEID.—This routine is called from a number of places and lists three items of information at the bottom of a page in the output listing and skips to a new page. The three items are (1) the name in columns 7-22 on the NAME records; (2) the word COEFFICIENTS if the page contains thermodynamic properties from least-squares coefficients or ORIGINAL if otherwise; and (3) either BAR or ATM to designate the standard reference unit of pressure as being either one bar or one atmosphere. PAGEID allows approximately 55 lines to be printed on a page. Up to six names from NAME records are saved and printed.

POLY.—This routine calculates thermodynamic functions for diatomic and polyatomic gases. It is called from the main program.

Subroutine INPUT is called from POLY to read the data records plus the next record. Subroutine LINK1 is called to calculate the partition function according to the method specified (RRHO, PANDK, JANAF, NRRAO1, or NRRAO2).

If more than one electronic state is present, the various states are identified by a code in columns 79 to 80 of the data records. In this case, data records for only one state at a time are read in and stored. The partition function for each state is calculated prior to processing data records for the next state.

PRINT.—This is one of five subroutines involved with internal rotation. This subroutine prints the number of energy levels and values of the potential function specified by NOUT (a label in a data record). It is called from IROTOR as an option only if NOUT is greater than zero.

PUNCH.—This routine writes on I/O units 6 and 10 the coefficients obtained either from a least-squares fit or from the data records associated with method COEF. PUNCH is called from subroutine DELH. See output details in appendix C.

QSUM.—This routine keeps a running total of all, except translational, contributions to the partition function and its derivative for each electronic state. These contributions are listed if an INTERM label has been included on the OUTPUT record. QSUM is called from a number of places in LINK1.

RECO.—The routine is called from the main program after reading a METHOD record which contains either a COEF or READIN label. The RECO routine calls INPUT to read the data records plus the next record.

For READIN, the temperature and the thermodynamic functions on each record are simply stored. For COEF, the thermodynamic functions are calculated for the temperatures on the temperature schedule and stored.

The RECO routine is also used to relate the enthalpy of two phases of the same species by means of an enthalpy or entropy of transition. One of these transition values is given on the

METHOD record of the second phase (DELTAH or DELTAS labels, see table VI) and used to calculate the enthalpy of the second phase at the transition temperature. The Gibbs energy value of the second phase is taken to be equal to the Gibbs energy value of the first phase at the transition temperature.

If a transition is present, the routine calls DELH (discussed in the section "DELH") to check for the options of least-squares fit or storing coefficients for the first phase.

TABLES.—This routine is called from the main program for printing the many-figured tables (MFIG on the OUTPUT record). It lists tables of thermodynamic functions for three sets of energy units for either *original* or *coefficients* data as discussed in appendix C. The format varies depending on the availability of the following values: (1) the $H_{298.15}^o - H_0^o$ value which is required in obtaining $H_T^o - H_{298.15}^o$ and $-(G_T^o - H_{298.15}^o)$, and (2) the H_0^o value which is required in obtaining H_T^o and $-G_T^o$.

TEMPER.—This routine stores the temperature schedules as given on TEMP or CTEM records. The TEMP records are for *original* data and CTEM for *coefficients* data. The routine is called from the main program after a TEMP record has been read and just before the *coefficients* tables are processed.

WCALC.—This is one of the two subroutines pertaining to the Wilhoit method of fitting thermodynamic data. It is called by subroutine WILHOI to calculate thermodynamic functions from Wilhoit coefficients.

WILHOI.—This is one of the two subroutines pertaining to the Wilhoit method of fitting thermodynamic data. It is used in PAC91 only for the purpose of extrapolation. WILHOI is

called in the main program if the label WILH has been included on a METHOD record. It generates the Wilhoit coefficients used in WCALC to extrapolate data. The desired temperature schedule for extrapolation is specified with TEMP input records.

BLOCK DATA.—BLOCK DATA contains the fundamental constants and information concerning chemical elements from hydrogen (atomic number 1) through californium (atomic number 98) and also electron gas and deuterium. These data consist of the following information for each element:

- (1) Chemical symbol
- (2) Atomic weight
- (3) Constant b in equation (8) or c^* for FILL option (see section **Inclusion of predicted levels**, and table I)
- (4) Sum of statistical weights for ground state (for FILL option)
- (5) Phase
- (6) Atomic number
- (7) Number of atoms in most abundant form of the element at room temperature

The atomic weights were taken from reference 50. The fundamental constants were taken from reference 10. The Sackur-Tetrode constant is given in equation (5). Other constants are as follows:

$$R = 8.31451 \text{ kJ/kg-mol-K}$$

$$c_2 = (hc/k) = 1.438769 \text{ cm-K}$$

Appendix A—Symbols

A_e, B_e, C_e	rotational constants corresponding to equilibrium separation of atoms	$\Delta_f H_T^o$	enthalpy of formation (heat of formation) of a substance at temperature T from its reference elements in their standard state
A_0, B_0, C_0	rotational constants for lowest vibrational state	$\Delta_{\text{trs}} H_T^o$	enthalpy of transition between two phases of a substance at temperature T
a_i	temperature coefficients in eq. (11)	$\Delta_{\text{trs}} S_T^o$	entropy of transition between two phases of a substance at temperature T
b	constant defined in eq. (8)	h	Planck constant
b_1	integration constant defined by eq. (12)	I_A, I_B, I_C	principal moments of inertia
b_2	integration constant defined by eq. (13)	J_i, J_m	total angular momentum quantum number
C_p^o	heat capacity at constant pressure for standard state	K	equilibrium constant
$C_p^o(0)$	heat capacity at constant pressure at 0 K	k	Boltzmann constant
$C_p^o(\infty)$	heat capacity at constant pressure at infinite temperature	L	total number of electronic energy states
c	velocity of light	ℓ	liquid phase of chemical substance
cr	crystal phase of chemical substance	M	molecular weight
c_2	second radiation constant, hc/k	m_μ	atomic mass constant
c^*	constant representing total quantum weight for each principal quantum number n above ground state n for some elements (see table I)	N	number of atoms in molecule
D_e	spectroscopic constants for rotational stretching	n	number of unique frequencies, number of phase angles, or principal quantum number
D_0, D_{000}	rotational stretching constants for lowest vibrational state	p_o	standard state pressure in eq. (5)
d_i	degeneracy associated with ν_i	Q	internal partition function
G_T^o	either $(G_T^o - H_0^o) + H_0^o$ or $(G_T^o - H_{298.15}^o) + H_{298.15}^o$	Q^m	internal partition function for m^{th} electronic state
$G_T^o - H_0^o$	Gibbs energy at temperature T relative to enthalpy at 0 K for standard state	Q_c^m	correction factor to the partition function for anharmonicity and vibration-rotation interaction for m^{th} electronic state
$G_T^o - H_{298.15}^o$	Gibbs energy at temperature T relative to enthalpy at 298.15 K for standard state	Q_e^m	electronic partition function for m^{th} electronic state
$\Delta_f G_T^o$	Gibbs energy of formation of a substance at temperature T from its reference elements in their standard state	Q_R^m	classical rotation partition function for m^{th} electronic state
g_i, g_m	electronic statistical weight	Q_V^m	harmonic-oscillator partition function for m^{th} electronic state
g_{ii}	anharmonicity constant for doubly degenerate vibrations in linear molecules	Q_W^m	Fermi resonance correction factor to partition function for m^{th} electronic state
H_0^o	chemical energy at 0 K for standard state	Q_θ^m	low temperature rigid rotational correction factor to partition function for m^{th} electronic state
$H_{298.15}^o$	assigned enthalpy at 298.15 K for standard state (equal to $\Delta_f H_{298.15}^o$)	Q_ρ^m	rotational-stretching—correction factor to partition function for m^{th} electronic state
H_T^o	either $(H_T^o - H_0^o) + H_0^o$ or $(H_T^o - H_{298.15}^o) + H_{298.15}^o$	q_i	temperature exponents in eq. (11)
$H_T^o - H_0^o$	sensible enthalpy at temperature T relative to 0 K for standard state	R	universal gas constant
$H_T^o - H_{298.15}^o$	sensible enthalpy at temperature T relative to 298.15 K for standard state	r	number of coefficients a_i in eq. (11)
		S_c	constant defined by eq. (5)
		S_T^o	entropy at temperature T for standard state

T	temperature, K	$\alpha_i^A, \alpha_i^B, \alpha_i^C, \alpha_{ij}$	vibration-rotation interaction constants for polyatomic molecules
T_0	electronic excitation energy between lowest vibrational states ($v = 0$) of ground and excited state for diatomic and polyatomic gases	β_i	rotational-stretching—vibration interaction constant
T_1	temperature, 1 K	ϵ_m	energy of m^{th} electronic state
u_i	$c_2\nu_i/T$	ν_i	observed fundamental frequency
V	potential	ρ	rotational-stretching spectroscopic constant
V_n	n -fold barrier	σ	symmetry number
v, v_i	vibrational quantum number	ω_e	zero-order vibrational frequency for diatomic molecule
W_0	Fermi resonance constant	$\omega_e x_e, \omega_e y_e, \omega_e z_e$	anharmonicity constants for diatomic molecules
x_{ij}, y_{ijk}	anharmonicity constants for polyatomic molecules		
α_e, α_i	vibration-rotation interaction constants for diatomic and linear polyatomic molecules		

Appendix B—Details in Preparing Input

Uniform Format

With a few exceptions, all input records are read in with an 80-column uniform format, namely A6, 4(A6, D12.0), I2. The exceptions are the formula, NAME and REFNCE records discussed in the section **Description of Input Records**. Another exception is EF data; however, EF data records are prepared by the program and not the user (see section **EFDA and EF data records**). The record columns for the uniform format are as follows:

	Record ID	Label 1	Numerical value 1	Label 2	Numerical value 2	Label 3	Numerical value 3	Label 4	Numerical value 4	
Record columns	1-6	7-12	13-24	25-30	31-42	43-48	49-60	61-66	67-78	79-80
Format	A6	A6	D12.0	A6	D12.0	A6	D12.0	A6	D12.0	I2

The labels (label 1, label 2, . . .) are codes on all types of input records except one. (The exception, described in the section **Data records for the FIXEDN, ALLN, or TEMPER methods**, is the record containing spectroscopic data for atoms.) These codes serve two purposes. One purpose is to specify an option in the program. For example, the label RRHO specifies a method of calculation. The second purpose is to identify the number which follows it. For example, the label STATWT precedes the numerical value of the statistical weight.

The last two columns (79 and 80) are used for several purposes:

(1) For atomic gases, the principal quantum numbers are put in these columns, right-adjusted, for methods FIXEDN and TEMPER. (See example 1 in appendix D.)

(2) For diatomic and polyatomic gases, the electronic level identification is put in these columns if excited states are included.

(3) For polyatomic gases with molecular data and internal rotors, the integers in these columns indicate the rotor to which the data belong.

(4) On the LSTSQS record, if different equations are used for different temperature intervals, the integer in column 80 indicates the interval associated with the information on the remainder of the record. Integers range from 1 to 8, with 1 assigned to the lowest temperature interval. (See example 1 in appendix D.)

Some general rules in preparing the input are as follows:

(1) With one exception, record ID's (columns 1 to 6) and labels are alphanumeric and must be left-adjusted. The exception is that the labels on the data records which contain spectroscopic constants for monatomic gases are numbers and

do not need to be left-adjusted. (See section **Data records** in this appendix and example 1 in appendix D.)

(2) All blank labels are ignored by the program.

(3) Each numerical value must be immediately preceded by its label. However, the order of values is usually immaterial. Exceptions are noted in the details for the individual records.

(4) The numerical values may be the following:

(a) A right-adjusted integer

(b) A floating-point number without exponent (e.g.,

0.00021), anywhere in the field

(c) A right-adjusted floating-point number with exponent indicating decimal place (e.g., 2.1-4 is 2.1×10^{-4})

(5) The last two columns (79 and 80) are right-adjusted integers.

Order of Input Records

Some discussion on the order of the input records is given in the section **General Flow of the Program**. Specific instructions for placement of the individual records are given in the details for preparing the records.

For a single computer run, there may be any number of species processed where each species requires its own set of input data. The set of input data records for each species should generally be in the following order:

(1) NAME record. While this record is optional, it is usually convenient to be first. Part of the contents of this record appears with least-squares coefficients output and also on the bottom of output listings. When there are multiple phases (indicated by two temperatures in the temperature schedule being adjacent and equal), there should be a corresponding NAME record for each phase. See example 8 in appendix D.

(2) Formula record (must be the first nonoptional record in the set)

(3) Miscellaneous records in any order containing options and information (namely, DATE, REFNCE, OUTPUT or CTEM)

(4) TEMP record(s), if any
(5) METHOD record
(6) Data record(s)
(7) FINISH record

} There may be more than one set of these records for a single species. (See examples 6 and 8, appendix D.)

There are two kinds of input records not directly related to input data sets, namely the LISTEF record and the EF data records.

Description of Input Records

Examples of the individual records discussed in this section are given in appendix D. All input records except the formula record are identified by a record ID (columns 1 to 6). However, PAC91 reads only the first four of the first six columns of the record ID. Six columns were reserved in order to provide a little more assistance in identifying the record. For example, the term METHOD is more descriptive than METH. However, either METH in columns 1 to 4 or METHOD in columns 1 to 6 is equally acceptable.

CTEM record.—The purpose of these records is to provide a temperature schedule for output tables generated from least-squares coefficients. However, the tables from coefficients will be printed only if the label CTAB is on the OUTPUT record. If no CTEM records are included in the input data set, the program will default to the temperature schedule of the original data. The labels associated with CTEM (T and I) and their corresponding numerical values have the same definitions as those used with the TEMP record. (See **TEMP record**.)

Data records.—These records follow the METHOD record and contain the input data required by the method. Except for the spectroscopic data of monatomic gases (see example 1, appendix D), the labels are codes identifying the numerical values that follow them. Table VII is a summary of the labels and numerical values to be used on data records for the various methods given in table VI. The data records may optionally contain identifying information in columns 1 to 6. For example, in the sample problems of appendix D, the species C_4H_4 (example 3) has the identifying word C4H4 in columns 1 to 6 of its data records. By contrast, columns 1 to 6 are blank for the species $Na_2CO_3(s)$ (example 8). However, whatever appears in columns 1 to 6 on the first data record, blank or otherwise, must also appear in columns 1 to 6 on all the remaining data records in the input data set. No data records are associated with METHOD WILH. A further description of the data records for various methods follows:

Data records for the READIN method: Generally, each record contains four labels with the four corresponding numerical values as indicated in table VII. The four labels correspond to temperature, heat capacity, enthalpy, and either entropy or Gibbs energy. Temperature, which must always be given, has the label T; however, for the other three properties there are several options of labels as given in table VII depending on the data to which they correspond. If enthalpy and Gibbs energy are referred to $H_{298.15}^0$ rather than H_0^0 , the $H_{298.15}^0 - H_0^0$ value must be included on the METHOD record (label H298H0) if $H_T^0 - H_0^0$ values are desired in the final tables. (See examples 6 and 8, appendix D.)

Sometimes one or two of the three properties are omitted in the data records or ignored by the PAC91 program. This

occurs when there are LSTSQS records that include one or two of the NOCP, NOH, or NOS labels. See **LSTSQS records**.

Data records for the COEF method: The coefficient and exponent values for each set of empirical equations (eqs. (11) to (13)) must be preceded by the values of the temperature limits (T labels in table VII) for which the equation applies (see examples 6 and 8, appendix D). The lower T value must be the first numerical value.

Occasionally the coefficients a_i ($i = 1, r$) are available while the integration constants for enthalpy and entropy b_1 and b_2 are not. For this case, b_1 and b_2 values may be calculated by the program in one of the following ways:

(1) Reading in an enthalpy and an entropy or Gibbs energy value with the corresponding temperature on the first record. The labels and values should be the same as for the data records for the READIN method except that C_p^0 or C_p^0/R may be omitted.

(2) Using the value of enthalpy or entropy of transition (DELTAH or DELTAS on the METHOD record (see table VI)). This method may be used only when the two phases related by the transition value are being processed in the same run. The reason is that the transition value is combined with the enthalpy or entropy value for the last temperature of the preceding phase. (See examples 6 and 8, appendix D.)

With the COEF method the TCOEF label provides an option to write these coefficients on I/O unit 10 in the same format as least-squares coefficients. (See table VIII.) For each set of coefficients, the temperature intervals may be specified in two different ways:

(1) If only the TCOEF label is given with no additional information on the record concerning temperature intervals, the temperature intervals will be taken from the T values accompanying the coefficient data (see Mg(l), example 6, and $Na_2CO_3(l)$, example 8, appendix D).

(2) Any temperature intervals may be specified by TCOEF labels and corresponding values which give the endpoints of the intervals. These values may or may not be the same as the T values for the set.

Data records for the FIXEDN, ALLN, or TEMPER methods: In contrast to all other types of records using the uniform format, these records use the label columns as well as the numerical columns for numbers. The labels contain either the total angular momentum quantum number J_m or the electronic statistical weight g_m (eq. (7)), and the numerical values contain the excitation energy ϵ_m/hc (eq. (7)) in centimeters⁻¹. If g_m values are used, the label GLABEL must be included on the METHOD record. For either the FILL option or the FIXEDN method, the principal quantum numbers must be included in columns 79 to 80, right-adjusted. The data on the remaining portion of the record must correspond to that principal quantum number. (See example 1, appendix D, for the TEMPER method and FILL option.)

Data records for the RRHO, PANDK, JANAF, NRRAO1, or NRRAO2 methods: The equations for the partition function

of the various methods are given in tables I and II. The input data must always contain at least the following quantities for each electronic state:

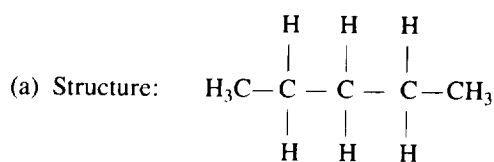
- (1) The fundamental vibrational frequencies of the molecule (ω_e or ν_i)
- (2) Either the rotational constant(s) (B_0 for linear; A_0 , B_0 , and C_0 for nonlinear molecules) or the moment(s) of inertia (I_B for linear; I_A , I_B , and I_C for nonlinear molecules)
- (3) The symmetry number
- (4) The statistical weight

Other spectroscopic constants such as anharmonicity or rotation-vibration interaction constants are optional. If these optional constants are not included, correction terms involving them are automatically excluded from the partition function. (See example 4 (RRHO), example 7 (JANAF), and example 5 (NRRAO2) in appendix D.)

When excited electronic states are involved, the data for each state are read and processed separately. Therefore, the data records must be grouped together with an identifying number in columns 79 to 80. For example, the data for the 15 electronic states included in example 7, appendix D, are distinguished by the integers 1 to 15 in columns 79 and 80.

Data records for the ADD method: The label and quantity for each of the appropriate groups forming the desired species must appear on these records. Example 2 in appendix D illustrates the ADD method. Table IX facilitates the preparation of the records inasmuch as it contains the PAC91 label notation, the Benson notation, the structure, the elements contained in the group, and the references for the selected thermodynamic data. The following two examples, for n-pentane and i-pentane (2-methyl butane), are given to further illustrate the use of this method:

(1) n-pentane

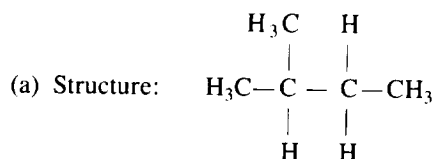


(b) Groups: 2CH_3 and 3CH_2

(c) Benson notation: $2\text{C}-(\text{H})_3(\text{C}) + 3\text{C}-(\text{H})_2(\text{C})_2$

(d) PAC91 record: (label number label number)
CH3C 2. CH2C2 3.

(2) i-pentane



(b) Groups: 3CH_3 , 1CH_2 , and 1CH

(c) Benson notation: $3\text{C}-(\text{H})_3(\text{C}) + \text{C}-(\text{H})_2(\text{C})_2$
 $+ \text{C}-(\text{H})(\text{C})_3$

(d) PAC91 record:

(label number label number label number)
CH3C 3. CH2C2 1. CHC3 1.
HRCO 402.6

The label HRCO on the second record is a correction term for the heat of formation due to the gauche interaction in i-pentane. Its value is obtained by dividing the value of 0.8 kcal/mole given in reference 36 by $R = 1.987216 \text{ cal/mol-K}$. Other terms used in the ADD method are given in table VII.

DATE record.—The purpose of the DATE record is to include a date and/or reference code with the least-squares coefficient output. The record should contain only one label which will be included in the second record of the least-squares coefficient output for each species. (See examples 1 to 4 and 6 to 8, appendix D.)

EFDA and EF data records.—The data on these records are used in conjunction with the LOGK option to obtain $\log_{10}K$ and $\Delta_f H_f^\circ$ values. These records are prepared automatically by the program when an EFTAPE label is included on the OUTPUT record of a reference element. For each reference element which has been processed in this manner one EFDA record and a varying number of EF data records are prepared depending on the amount of thermodynamic data available for each reference element. The combination of the one EFDA record and EF data records which follow it will be referred to as EF data. The contents of an EFDA record consists of the chemical formula of the EF data reference element, the date code, the H_0°/R value, the melting point, if any, and the number of temperatures for which there are enthalpy and Gibbs energy values following the EFDA record. Each EF data record consists of a temperature (K), an enthalpy $(H_T^\circ - H_0^\circ)/RT$ value, and a Gibbs energy $-(G_T^\circ - H_0^\circ)/RT$ value followed by a second temperature, enthalpy, and Gibbs energy. A listing of typical EF data for an element is shown in the output for Mg(s,l), example 6, appendix D.

Additional discussion of EF data sets is given in the section **Saved Output** in appendix C.

FINISH record.—This required record is the last record in the input set for each species. It contains only the code FINISH in columns 1 to 6.

Formula record.—This is the first nonoptional record in the input data set for each species and is reserved for two pieces of information. First, the species formula, as detailed below, is always required. Second, either an assigned enthalpy or a heat of reaction value with the corresponding units and temperature is required only if the assigned enthalpy column (H_T° or H_T°/R) is desired in the output tables, or when calling

for either of the following two options:

- (1) $\log_{10}K$ and $\Delta_f H_f^\circ$ calculations (also requires a LOGK label on an OUTPUT record), or
- (2) Least-squares fit of the thermodynamic functions (also requires a LSQS label on an OUTPUT record)

All the examples in appendix D, with the exception of C_2H_3 (example 2), have either an assigned enthalpy ASINDH or a heat of formation HF298. C_2H_3 uses METHOD ADD which calculates the heat of formation.

The first 12 columns are reserved for the formula of the species. The formula should be left-adjusted and contain no blanks. It should be prepared in the following order:

- (1) Each atomic symbol followed by the number of atoms even if the number is 1; these atomic symbols should all be in capital letters and correspond to the symbols in BLOCK DATA.
- (2) For ionic species, the proper number of pluses or minuses
- (3) For condensed species, a left parenthesis
- (4) For condensed species other than reference elements, any character except G (e.g., an L for a liquid, an S for solid, or C for crystal)
- (5) For condensed species to be used as reference elements, the character must be S for solid or L for liquid (in order to match the formula in BLOCK DATA).
- (6) For condensed species, a right parenthesis

The following are some examples, primarily for ionized species:

Species	Columns 1 to 12
$CaCO_3(s)$	CA1C1O3(S)
F^-	F1-
N^+	N1+
O^{++}	O1++
O_2	O2-

The remainder of the record is reserved for a heat of formation, the energy units, and the temperature of the reaction. There are three forms in which the heat of formation may be expressed and six choices of units. These are summarized in table V.

LISTEF record.—This option is used to obtain a listing of the EF data stored on I/O unit 13.

LSTSQS record.—No least-squares calculations will be made without a LSQS label on the OUTPUT record. By contrast, the LSTSQS record is required only for specifying any of the nonstandard (or non-default) options pertaining to the least-squares fit of the functions C_p°/R , H_f°/RT , and S_f°/R to equations (11) through (13). The options are summarized in table IV.

With a LSQS label and no LSTSQS record, the program will attempt the default options. They include the following:

- (1) Fitting the three functions simultaneously
- (2) Setting the q_i values in equation (11) to be -2 , -1 , 0 , 1 , 2 , 3 , and 4

- (3) Setting two temperature intervals, 200 to 1000 and 1000 to 6000 K
- (4) Constraining the fit to fit the three functions exactly at 298.15 K
- (5) Constraining the fitted functions to match at 1000 K (The coefficients for the higher temperature interval are constrained to reproduce the fitted results of the lower temperature interval at 1000 K.)

If an OLD label is listed on the LSTSQS record, the default q_i values in equation (11) change to 0, 1, 2, 3, and 4, to match the *old* polynomial form used for C_p° in reference 41.

If a NOCNS label is given, the fit is not constrained to fit any values of the functions. The fit may be constrained to fit the functions exactly at a specified temperature provided the temperature is in the temperature schedule of the data. This temperature value follows a TCONST label. In this case any common points between any succeeding intervals will be constrained to match.

The temperature intervals may be changed by using T labels, each followed by one value (namely, the first temperature, the breakpoints, and the final temperature, all in kelvin). The program will order these values from the lowest to the highest. Allowance is made for up to 8 intervals (9 values).

The q_i values in equation (11) may be set with EXP labels. These exponent values may be positive, negative, zero, or fractional. As always, the integers following a label must include a decimal point. The program orders these values from the lowest to the highest. The limit on the number of exponents (r in eq.(11)) is 8. Different sets of EXP values may be used for different temperature intervals by giving the appropriate temperature interval number in column 80 (with 1 referring to the lowest interval). If a set of EXP values is given without specifying an interval (i.e., column 80 is blank), this set will be used for all unspecified intervals. If there is no EXP set given with column 80 blank, the default set will be used for the unspecified intervals.

For fitting one function only or some combination of two functions the labels NOCP (no C_p°), NOH (no H_f°), and NOS (no S_f°), are provided. The labels are used as follows:

Functions to be fit simultaneously	Label on LSTSQS record
C_p°/R only	NOH and NOS
H_f°/RT only	NOCP and NOS
S_f°/R only	NOCP and NOH
C_p°/R and H_f°/RT	NOS
C_p°/R and S_f°/R	NOH
H_f°/RT and S_f°/R	NOCP

With NOS and NOH combinations, an enthalpy value is required to obtain the b_1 integration constant and an entropy value is required to obtain the b_2 constant. In this case, a TPROP label with its corresponding temperature is required on the record. PAC91 then expects to find the required

properties at this temperature in the data obtained from the METHOD and data records. When NOCP, NOH, or NOS labels are used, it is assumed these data (C_p^o , H_T^o , or S_T^o) for the remaining temperatures are either missing or wrong. PAC91 will fill these data with the values it gets from the least-squares fit, even for the *original* tables. These simultaneous fit combinations may vary between temperature intervals using the same method described above for the functional form. The temperature interval number is put in column 80 on the LSTSQS records with the appropriate parameters.

METHOD record.—This record follows the option records and must be included for any calculations to take place. It specifies the technique for obtaining the thermodynamic functions (see section **Options**) and immediately precedes the data required by the method (data records). The record has the code word METHOD in columns 1 to 6. The possible codes in the label and numerical value columns are summarized in table VI. The functions may be (1) calculated from molecular constants for ideal gases (labels FIXEDN, ALLN, or TEMPER for monatomic molecules and labels RRHO, PANDK, JANAF, NRRAO1, or NRRAO2 for diatomic and polyatomic molecules) (see examples 1, 4, 5, and 7, appendix D); (2) calculated from coefficients and exponents using equations (11) to (13) (label COEF), (see examples 6 and 8, appendix D); (3) read in directly (label READIN) (see examples 3, 6, and 8, appendix D); (4) estimated by a group additivity method (label ADD) (see example 2, appendix D); or (5) extrapolated functions using the Wilhoit method (label WILH, see examples 2 and 3, appendix D). The calculation techniques listed in (1) are discussed in the section **Calculation of Ideal Gas Thermodynamic Functions**.

In conjunction with these method labels, the METHOD record may contain some additional labels and information as indicated in table VI.

Occasionally, a single method may not apply to the entire desired temperature range for a species. In this case the following records must be included for each temperature interval, in order: (1) TEMP record(s) for the desired temperature interval (if the method is not READIN), (2) a METHOD record for this temperature interval, and (3) the associated data records. The sets should be in order of increasing temperature. (See examples 2, 3, 6 and 8, appendix D.)

The WILH method always follows another method and requires no data records to follow it. This method generates Wilhoit-fit coefficients in order to extrapolate thermodynamic data obtained from the previous method to higher temperatures. The temperature schedule for the extrapolation must be specified with TEMP records immediately preceding the WILH method record. If the species is linear, the label LINE must be specified (otherwise the default is to nonlinear).

NAME record.—This record contains a name and comments. PAC91 allows for up to six NAME records in a data set for a species. For least-squares coefficients, one name and associated comments are transferred to the output for each set of

coefficients. Columns 7-24 are used for the name and columns 25-80 are used for comments (see table VIII).

Multiple NAME records are useful in identifying multiple phase or lambda transitions for condensed species. When PAC91 encounters the same temperature in two adjacent slots in the temperature schedule, it assumes there will be a new set of coefficients using the name and comments from the next NAME record, if there is one. If there is not, it uses the name and comments from the previous NAME record (see examples 6 and 8, appendix D).

OUTPUT record.—The OUTPUT records contain options for output. There are 10 possible labels for this purpose and no numerical values. These labels (options) are now summarized:

ATM label. Calls for pressure to be in units of atmospheres in the entropy and Gibbs energy values appearing in the output tables. The default units are bars.

CAL label. Calls for tables with calories as the energy units. The label must be combined with either MFIG or LOGK or both.

CTAB label. Calls for tables of functions calculated from coefficients to be printed. The label must be combined with either MFIG or LOGK or both.

DMLESS label. Calls for many-figured tables in dimensionless units.

EFTAPE label. Used with an assigned reference element whose data are needed for $\Delta_f H_T^o$ and $\log_{10} K$ calculations. Inclusion of the label causes the H_0^o value and the $(H_T^o - H_0^o)/RT$ and $-(G_T^o - H_0^o)/RT$ data for this species to be merged with the EF data on I/O unit 13 in unformatted form. These functions are also written on I/O unit 11 in formatted form. See example 6, appendix D.

INTERM label. Calls for intermediate output to be printed when thermodynamic functions are being calculated from molecular constants. (See section **Intermediate data with INTERM label**, appendix C and example 5, appendix D.)

JOULES label. Calls for tables with joules as the energy units. The label must be combined with MFIG or LOGK or both.

LOGK label. Causes rounded tables of thermodynamic properties including $\Delta_f H_T^o$ and $\log_{10} K$ to be listed. If no units label is specified, JOULES will be assumed. If the appropriate EF data are not available on I/O unit 13, the $\Delta_f H_T^o$ and $\log_{10} K$ columns will be left blank. If there is no matching temperature in the assigned reference element data, the data that are there will be interpolated by three-point Lagrangian interpolation. (See example 8, appendix D.)

LSQS label. Calls for a least-squares fit of the functions to equations (11) to (13). Unless otherwise specified on the LSTSQS record, the q_i values assigned will be -2, -1, 0, 1, 2, 3, and 4. If no T's are given, the temperature intervals assigned will be 200 to 1000 K and 1000 to 6000 K. For condensed species, transition points are automatically inserted.

MFIG label. Causes many-figured (unrounded) tables of functions to be printed. If no energy unit label is given, JOULES will be assumed.

REFNCE record.—The only purpose of this record is for comments such as identifying sources of input data. All the information in columns 7-80 in this record is alphanumeric. The usual labels and numerical values are ignored. (See examples 1, 3, 4, and 6, appendix D.)

TEMP record.—These records give a temperature schedule for which thermodynamic functions are to be calculated. The program allows for a maximum of 202 temperatures per species.

Each temperature in the desired temperature schedule may be specified individually with a T label. (See table IV.) However, if there are several temperatures incremented by a fixed amount, this part of the temperature schedule may be specified by giving, in order, the lowest temperature labeled T, the increment labeled I, and the highest temperature labeled T. For example, the temperature schedule, 100, 200, 298.15, 300, 400, 500, 600, 688.2, 700, 750, 800, 850, 900, 962.3, and 1000, could be designated as follows:

The temperature 298.15 K is always inserted in the temperature schedule automatically by PAC91 when there are temperature values below and above 298.15 K. (See examples 1 and 4, appendix D.)

If there are no TEMP records in a set of data where the thermodynamic functions are to be calculated, the program assumes the standard temperature schedule used in reference 4—namely, every 100 K from 100 to 6000 K with 298.15 K inserted between 200 and 300 K. (See example 7, appendix D.)

TEMP records should not precede METHOD records with READIN. For this option, the temperatures are read in on the data records together with the thermodynamic functions to which they correspond. (See examples 3, 6, and 8, appendix D.)

Record ID	Label 1	Numerical value 1	Label 2	Numerical value 2	Label 3	Numerical value 3	Label 4	Numerical value 4
TEMP	T	100.	I	100.	T	600.	T	688.2
TEMP	T	700.	I	50.	T	900.	T	962.3
TEMP	T	1000.						

Appendix C—Details in Output

Listed Output

Input data in the uniform format as well as some intermediate data are listed for each set of input. Other tables and data will be listed according to the options on the OUTPUT record.

Input data.—All input data in the uniform format are listed immediately after they are read in the same format. Numerical values which are zero may be left blank. (See examples in appendix D.)

Tables of original thermodynamic properties.—(See section **Output** for discussion of original data and data from least-squares coefficients.) There are 10 possible tables printed according to the labels on the OUTPUT record, five for *original* data and a corresponding five for data calculated from least-squares coefficients. In each set of five tables, there are three possible many-figured tables (label MFIG) and two possible rounded tables with $\Delta_f H_T^\circ$ and $\log_{10} K$ columns (label LOGK). These tables vary with units: (1) dimensionless with DMLESS label (for many-figured tables only); (2) SI units with a JOULES label; and (3) energy units in calories with the CAL label. The properties in these tables are the following:

(1) In dimensionless form—

T , C_p°/R , $(H_T^\circ - H_0^\circ)/RT$, $(H_T^\circ - H_{298.15}^\circ)/RT$ (if $T = 298.15$ K is in T range), S_T°/R , $-(G_T^\circ - H_0^\circ)/RT$, $-(G_T^\circ - H_{298.15}^\circ)/RT$ (if $T = 298.15$ K is in T range), and H_T°/RT and $-G_T^\circ/RT$ (if an H_0° value is available)

(2) In dimensioned, many-figured form—

T , C_p° , $H_T^\circ - H_0^\circ$, $H_T^\circ - H_{298.15}^\circ$ (if $T = 298.15$ K is in T range), S_T° , $-(G_T^\circ - H_0^\circ)$, $-(G_T^\circ - H_{298.15}^\circ)$ (if $T = 298.15$ K is in T range), and H_T° and $-G_T^\circ/RT$ (if an H_0° value is available)

(3) In dimensioned, rounded figure form—

T , C_p° , $H_T^\circ - H_{298.15}^\circ$ (if $T = 298.15$ K is in T range), S_T° , $-(G_T^\circ - H_{298.15}^\circ)$ (if $T = 298.15$ K is in T range), H_T° , and $\Delta_f H_T^\circ$ and $\log_{10} K$ for formation from assigned reference elements

These tables will have an asterisk and a footnote indicating where a phase transition has occurred in an assigned reference element. (See example 8, appendix D.)

All five of the tables containing original data have the word ORIGINAL on the bottom of each page.

Tables of thermodynamic properties from least-squares coefficients.—If a CTAB label is included on an OUTPUT record, tables of properties calculated from least-squares coefficients will be listed. These tables will have the same

format as the *original* tables described in the previous section for the same labels on the OUTPUT records. They may be differentiated from the tables of *original* data by the word COEFFICIENTS on the bottom of each page. The temperature schedule for these tables may be changed from the input temperature schedule by the use of CTEM records.

Tables of least-squares errors.—A least-squares fit of the functions C_p°/R , $(H_T^\circ - H_0^\circ)/RT$, and S_T°/R results when a LSQS label is included on the OUTPUT record. (See examples 1, 6, 7, and 8 in appendix D.)

For each temperature interval, the following information is listed:

- (1) For each T within the interval,
 - (a) C_p°/R , $(H_T^\circ - H_0^\circ)/RT$, S_T°/R , and $-(G_T^\circ - H_0^\circ)/RT$
 - (b) Functions in (1a) above as calculated from least-squares coefficients and equations (11) to (13)
 - (c) Differences in (1a) and (1b); these values are referred to as errors hereinafter
 - (d) Values in (1c) divided by original values in (1a); these values are referred to as relative errors hereinafter
- (2) For errors in entire interval for each function in (1a):
 - (a) Maximum relative error (MAX REL ERR) and corresponding temperature—see (1d)
 - (b) Average relative error (AVER REL ERR)—see (1d)
 - (c) Root mean square of relative errors (REL LST SQ ERR)—see (1d)
 - (d) Maximum error (MAX ERR) and corresponding temperature—see (1c)
 - (e) Average error (AVER ERR)—see (1c)
 - (f) Root mean square of errors (LST SQ ERR)—see (1c)
 - (g) C_p°/R equation (see eq. (11)) for coefficients a_i
 - (h) Integration constants in equations (12) and (13) as follows:

$$(H - H_0)/R \text{ CONSTANT} = b_1 - H_0^\circ/R$$

$$H/R \text{ CONSTANT} = b_1$$

$$S/R \text{ CONSTANT} = b_2$$

Finally, the contents of the least-squares coefficient records are listed on I/O unit 10 as well as on I/O unit 6. See the section **Output** and table VIII.

EF data.—These data, which contain the enthalpy and Gibbs energy data for reference elements, will be listed for two situations. First, they will be listed when a reference element is being processed and there is an EFTAPE label on the OUTPUT record. The data, in dimensionless form, are written on I/O unit 11 as well as on I/O unit 6 (see example 6, Appendix D for a listing of EF data for a reference element). The data are also merged in the library of unformatted data on I/O unit 13 (see **Saved Output**). Secondly, a LISTEF record will cause all unformatted data on I/O unit 13 to be listed.

Intermediate data with FILL option for monatomic gases.—Unobserved but predicted energy levels for monatomic gases will be included in the partition function (eq. (7)) if the FILL code is included in the METHOD record. See the section **Inclusion of predicted levels** for the method of predicting the levels.

In argon (example 1, appendix D), the following data are listed in columns from left to right (refer to eq. (8) and table I):

- (1) b value
- (2) Principal quantum number n
- (3) bn^2 or c^* [predicted $\sum (2J_i + 1)$]
- (4) $\sum (2J_i + 1)$ from input data
- (5) Column (3) minus column (4)
- (6) Highest energy level for principal quantum number
- (7) Sum of column (5) and $2J_i + 1$ for level of column (6)

Intermediate data with INTERM label.—Intermediate data are listed for ideal gas calculations if an INTERM label is included on the OUTPUT record for a particular species.

Monatomic gases: For monatomic gases several items are listed. The input data are listed in order of increasing energy level values. The data include, from left to right, values for the principal quantum number n , J_i , $2J_i + 1$, and the energy level.

For each temperature, three lines of data are listed as follows:

(1) A statement indicating where the energy levels were cut off; five possible statements are the following:

(a) NOT ALL LEVELS WERE USED. X IS GREATER THAN 85.—This statement indicates that not all atomic energy levels were used because $\epsilon/kT > 85$ in equation (7).

(b) ALL LEVELS USED THROUGH N = (FIXEDN value)—This statement indicates all atomic levels were used through a fixed principal quantum number (method FIXEDN).

(c) ALL ASSIGNED LEVELS HAVE BEEN USED—This statement indicates all atomic levels in input were used (method ALLN).

(d) NOT ALL ASSIGNED LEVELS WERE USED, Q AND DERIVATIVES ARE TOO SMALL—This statement indicates not all atomic levels were used because the following conditions occurred:

$$Q^m \leq 1 \times 10^{-10}$$

and

$$(\epsilon_m/kT)^2 Q^m \leq 1 \times 10^{-10}$$

when $\epsilon_m/kT > 2$.

(e) ALL LEVELS HAVE BEEN USED TO THE THERMAL BINDING ENERGY—This statement gives the lowered ionization potential value (i.e., ionization potential— kT/hc) where energy levels with higher values have been cut off.

- (2) Values of T , C_p^o/R , $(H_T^o - H_0^o)/RT$, and $-(G_T^o - H_0^o)/RT$

- (3) Values of ϵ/kT , Q , $T dQ/dT$, $T^2 d^2Q/dT^2 + 2T dQ/dT$

Diatomic and polyatomic gases: Intermediate results are listed when an INTERM record is included in the input data set for a diatomic or polyatomic gas and the method of calculation is RRHO, JANAF, PANDK, NRRAO1, or NRRAO2. These results include values for the formulas and variables defined in tables II and III. Although the molecular constants are always listed as they appear in the data records, with an INTERM record many of them are listed again.

The following data are listed (see tables II and III for definitions and $H_2O(g)$ in example 5, appendix D):

- (1) a_i , α_i^A , α_i^B , α_i^C where $i = 1$ to the number of unique frequencies
- (2) θ_1 , θ_2 , θ_3
- (3) A_0 , B_0 , C_0 , ρ
- (4) y_{ijk}
- (5) x_{ij}
- (6) LEVEL = (value in record columns 79 to 80 which is used to identify the electronic levels)
- (7) v_i , d_i , g_{ii}
- (8) T
- (9) u_i , r_i , s_i , i

(10) As required by the method of calculation, values for the formulas in tables II and III are listed for Q , $\ln Q$, $T d(\ln Q)/dT$, and $T^2 d^2(\ln Q)/dT^2 + 2T d(\ln Q)/dT$. The latter three values are additive contributions to $-(G_T^o - H_0^o)/RT$, $(H_T^o - H_0^o)/RT$, and C_p^o/R , respectively, when only the ground electronic state is considered. These values are identified in the listing by codes which correspond to the formula numbers as follows:

Code on listing	Formula numbers in tables II and III
ELEC	1
H.O.	2
R.R.	3 or 4
RHO	5
THTA	6
FERM	7
ALFA	8 to 11
XIJ	12 or 14
YUK	13
G+AG	16
WEZE	15
AXIJ	17
XIJ2	18 and 19
XY	20 and 21
G2GX	22 and 23
AX2	24 to 27

Saved Output

As previously mentioned (see section **Computer Program**), some of the options require I/O units 10, 11, 13, 14, 17, and 19 in addition to the standard I/O units 5 and 6. I/O units 14 and 17 are scratch formatted and unformatted output units respectively for EF data processing. The other I/O units

contain data that may be saved for various purposes as summarized in the following table. More details are given in the following sections.

I/O unit ^a	Option		Contents	Format	I/O type
	Record ID	Label			
10	OUTPUT	LSQS	Coefficients (Groups and Species)	Formatted (table VIII)	Output
19	METHOD	ADD	Coefficients (Group)	Formatted (table VIII)	Input
13	OUTPUT	EFTAPE	EF data ^b	Unformatted	Output
11	OUTPUT	EFTAPE	EF data ^b	Formatted	Output
13	OUTPUT	LOGK	EF data ^b	Unformatted	Input
5	EFDA	(element)	EF data ^b	Formatted	Input

^aNote that some of the input data (I/O units 19, 13, and 5) used by PAC91 were also produced by PAC91 (I/O units 10, 13, and 11).

^bReference elements.

The coefficients for a group written on I/O unit 10 have to be moved to the file associated with I/O unit 19 for future use. On the other hand, when an EFTAPE label is included on the OUTPUT record for a reference element, the EF data are automatically inserted in the unformatted data on I/O unit 13 for immediate use. The data are also written in formatted form on unit 11 which may be moved to a file as a backup. This file

may be read in on I/O unit 5 and the program will put the data on I/O unit 13. The LISTEF record simply lists the data from I/O unit 13 so that they may be checked if so desired.

EF data.—For every reference element processed by PAC91 which includes an EFTAPE label on the OUTPUT record, the EF data which are generated are stored in I/O unit 11 in formatted form and in I/O unit 13 in unformatted form. (See example 6, appendix D, for a typical EF data set.) I/O unit 11 is used to store these data for just the reference elements currently being processed. I/O unit 13, by contrast, is used to include these data with EF data for all reference elements previously processed. If the current element has the same name as an element previously stored on I/O unit 13, the previously stored data for that element will be replaced by the current data. The formatted data on I/O unit 11 may be moved to another file and saved if desired. There are three reasons for doing this: (1) the data are legible, (2) they can serve as a backup since PAC91 can read in the data on I/O unit 5 and write it out on I/O unit 13, and (3) they are more easily transported to other computer systems.

Least-squares coefficients.—The least-squares coefficients are written in the file associated with I/O unit 10. The format is described in table VIII. Generally these data will be for use in other computer programs (e.g., ref. 41). These coefficients may also be for a group and used by PAC91 for the group additivity method (METHOD ADD). For this latter case, the coefficients must be transferred from I/O unit 10 to the file of data associated with I/O unit 19.

Appendix D—Examples

Eight sample problems were selected to illustrate a number of the methods, features, and options of PAC91. Both input and output are given in these examples. To conserve space, the output has been deliberately kept short by using shorter temperature schedules than would normally be used. For example, only one temperature, $T = 5000$ K, is given for H_2O due to the large amount of intermediate output.

In addition to the H_2O intermediate output several other types of intermediate output are also illustrated. These will be discussed for the appropriate examples.

The following methods are illustrated for the species shown:

Method	Species	Example numbers
ADD	C_2H_3	2
COEF	$\text{Mg}(\ell)$, $\text{Na}_2\text{CO}_3(\ell)$	6,8
JANAF	MgO	7
NRRAO2	H_2O	5
READIN	C_4H_4 , $\text{Mg}(\text{s})$, $\text{Na}_2\text{CO}_3(1,2)$	3,6,8
RRHO	C_5H_{11}	4
TEMPER	Ar	1
WILH	C_2H_3 , C_4H_4	2,3

The required records—namely, the formula, OUTPUT, METHOD, data and FINISH records—appear in each example. The optional NAME, DATE, REFNCE, TEMP, and CTEM records as well as a number of other records and labels are also illustrated in the following examples.

Example 1. Ar(g) from Method TEMPER with FILL and LSQS Options

Problem.—Calculate and print thermodynamic functions to 20 000 K for Ar using method TEMPER with FILL option and obtain a least-squares fit of the calculated data. Print tables of functions, both original data and data from least-squares coefficients, in the three options of energy units and the many-figured form.

The standard I/O unit 5 input and the standard I/O unit 6 output are listed below.

For the input, the record names were all limited to four characters except the FINISH record. The number of and names of these records are, in order: 1 NAME, 1 formula, 1 DATE, 1 REFN, 2 TEMP, 5 LSTS, 2 OUTP, 1 METH, 35 data, and 1 FINISH. The NAME record gives the name of the species and, for the comments portion, the data reference

and method of calculation. The formula record gives the species formula in capital letters for the alphabetic part, the stoichiometric coefficient of 1, and the assigned enthalpy of 0 at 298.15 K (HF298). The DATE record contains a code chosen to stand for Lewis, June 1988—namely, L 6/88. The REFN record gives more information regarding the reference for the spectroscopic data. The TEMP records give the temperature schedule—namely, 100 and 500 and 1000 to 20 000 K in 1000 K increments. The first LSTS record gives the temperature interval endpoints for the least-squares fit—namely, 298.15, 1000, 6000, and 20 000 K. The second and third LSTS records give just one $\text{EXP} = 0$ value (q_i in eq. (11)) for temperatures intervals 1 and 2 (given in column 80). This is because C_p^o/R is a constant in these temperature ranges. The last two LSTS records give seven exponent values for the third interval (6000 to 20 000 K).

No least-squares fitting will take place and no tables printed unless these options are listed on the OUTP records. In this case, the options include many-figured tables (MFIG) in three sets of energy units (DMLESS, JOULES, and CAL), a least-squares fit (LSQS), and tables from the least-squares coefficients (CTAB). Specified energy units apply to both original and least-squares tables.

The METH record indicates the temperature cutoff method (TEMPER) with the missing levels filled in (FILL). The data records, which are identified by AR in columns 1 and 2, contain energy levels and corresponding J_m values. The principal quantum numbers 3 through 14 to which these energy levels belong are required by FILL and are given in columns 79 and 80. The J_m values are found in the label portions of the records. Note that these values may be anywhere in the label columns and integers do not require decimal points. The last data record contains the ionization potential (IP) needed for the temperature cutoff method.

The first part of the listed output is simply a copy of the input records except for the atomic weight which is inserted after the METH record. The seven columns of information following the FINISH record are related to the FILL option. These are described in appendix C under **Intermediate data with FILL option for monatomic gases**. Similarly, the least-squares output is detailed in the section **Tables of least-squares errors**. The remaining tables result from the remaining labels on the OUTP record—namely, DMLESS, JOULES, CAL, MFIG, and CTAB. Again refer to the appendix C sections **Tables of original thermodynamic properties** and **Tables of thermodynamic properties from least-squares coefficients**.

Input. - The input data set for Ar, example 1, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79 80
a NAME	Argon		NSRDS	NBS 35, 1971	Temperature cutoff & FILL			Expl.	1
ARI			HF298	0.					
DATE	L 6/88								
a REFN	MOORE,	ATOMIC ENERGY LEVELS, NSRDS-NBS 35, 1971, PP 211-215.							
TEMP	T	100.	T	500.	T	1000.	I	1000.	
TEMP	T	20000.							
LSTS	T	298.15	T	1000.	T	6000.	T	20000.	
LSTS	EXP	0.							1
LSTS	EXP	0.							2
LSTS	EXP	0.	EXP	1.	EXP	2.	EXP	3.	3
LSTS	EXP	4.	EXP	-1.	EXP	-2.			3
OUTP	MFIG		DMLESS		JOULES		CAL		
OUTP	LSQS		CTAB						
METH	TEMPER		FILL						
AR	0	0.	0	111667.87					3
AR	1	111818.09	4	112750.22	3	113020.39	2	112138.98	3
AR	1	114147.75	2	113426.05	3	113716.61	2	114641.04	3
AR	3	114831.99	2	114805.18	1	115366.9			3
AR			2	93143.8	1	93750.639	0	94553.707	4
AR	1	95399.87	1	104102.144	3	105462.804	2	105617.315	4
AR	1	106087.305	2	106237.597	0	107054.319	1	107131.755	4
AR	2	107289.747	1	107496.463	0	108722.668			4
AR	0	118512.17	1	118651.447	4	119023.699	3	119212.93	4
AR	2	118906.665	1	119847.81	2	119444.88	3	119566.11	4
AR	2	120619.076	3	120753.52	2	120600.944	1	121011.979	4
AR	1	120188.34	2	120188.66	5	120207.32	4	120207.77	4
AR	3	120229.81	2	120230.07	7.5	120250.15	13.5	121654.	4
AR	2	113468.55	1	113643.26	0	114861.67	1	114975.07	5
AR	1	116660.054	3	116942.815	2	116999.389	1	117151.387	5
AR	2	117183.654	0	117563.020	1	118407.494	2	118469.117	5
AR	1	118459.662	0	118870.981	0	121794.158	1	121932.908	5
AR	10	122090.	1	122514.29	5.5	122310.	5.5	123535.	5
AR	2	123372.987	1	123815.53	27.5	122700.	13.5	124137.	5
AR	2	119683.113	1	119760.22	0	121096.67	1	121161.356	6
AR	11.5	121205.	5.5	122633.	19.5	123741.	9.5	125140.	6
AR	27.5	124050.	13.5	125483.					6
AR	3.5	122455.	1.5	123880.	11.5	123230.	5.5	124660.	7
AR	19.5	124652.	9.5	126069.	27.5	124863.	13.5	126295.	7
AR	11.5	124400.	5.5	125800.	19.5	125280.	27.5	125390.	8
AR	3.5	123920.	1.5	125340.					8
AR	3.5	124780.	1.5	126210.	11.5	125100.	1.5	126524.2	9
AR	19.5	125650.	3.5	127130.	27.5	125754.			9
AR	3.5	125330.	11.5	125540.	19.5	125940.	3.5	127410.	10
AR	3.5	125712.	1.5	127130.	5.5	125860.	19.5	126155.	11
AR	3.5	127610.							11
AR	7.5	126000.	19.5	126300.	3.5	127760.			12
AR	5.5	126200.	1.5	127610.	19.5	126430.	3.5	127880.	13
AR	3.5	126330.	1.5	127600.	19.5	126520.	3.5	127970.	14
AR	IP	127109.9							
FINISH									

^aAll alphanumeric characters.

Listed output. - The listed output for Ar, example 1, is as follows:

```

NAME Argon          NSRDS-NBS 35, 1971. Temperature cutoff & FILL.  Expt. 1
ARI                HF298  0.
DATE  L 6/88
REFN  MOORE, ATOMIC ENERGY LEVELS, NSRDS-NBS 35, 1971, PP 211-215.
TEMP  T    100.    T    500.    T    1000.    I    1000.
TEMP  T    20000.
LSTS  T    298.15  T    1000.    T    6000.    T    20000.
LSTS  EXP    0.                                1
LSTS  EXP    0.                                2
LSTS  EXP    0.    EXP    1.    EXP    2.    EXP    3.    3
LSTS  EXP    4.    EXP    -1.    EXP    -2.    3
OUTP  MFIG      DMLESS      JOULES      CAL
OUTP  LSQS      CTAB
METH  TEMPER      FILL
ATOMIC WEIGHT = 39.94800
AR    0      0.    0      111667.87                                3
AR    1      111818.09  4      112750.22  3      113020.39  2      112138.98  3
AR    1      114147.75  2      113426.05  3      112716.61  2      114641.04  3
AR    3      114831.99  2      114805.18  1      115366.9                                3
AR    2      95143.8    1      93750.639  0      94553.707  4
AR    1      95599.87  1      104102.144  3      105462.804  2      105617.315  4
AR    1      106087.305  2      106237.597  0      107054.319  1      107131.755  4
AF    2      107289.747  1      107496.463  0      108722.668                                4
AF    0      118512.17  1      118651.447  4      119023.6993      119212.93  4
AR    2      118906.665  1      119847.81  2      119444.88  3      119566.11  4
AR    2      120619.076  3      120753.52  2      120600.944  1      121011.979  4
AR    1      120188.34  2      120188.66  5      120207.32  4      120207.77  4
AR    3      120229.81  2      120230.07  7.5      120250.15  13.5      121654.    4
AR    2      113468.55  1      113643.26  0      114861.67  1      114975.07  5
AR    1      116660.054  3      116942.815  2      116999.389  1      117151.387  5
AR    2      117183.654  0      117563.020  1      118407.494  2      118469.117  5
AR    1      118459.662  0      118870.981  0      121794.158  1      121932.908  5
AR    10     122090.    1      122514.29  5.5      122310.    5.5      123335.    5
AR    2      123372.987  1      123815.53  27.5      122700.    13.5      124137.    5
AR    2      119683.113  1      119760.22  0      121096.67  1      121161.356  6
AR    11.5    121205.    5.5      122633.    19.5      123741.    9.5      125140.    6
AR    27.5    124050.    13.5      125483.                                6
AR    3.5     122455.    1.5      123880.    11.5      123230.    5.5      124660.    7
AR    19.5    124652.    9.5      126069.    27.5      124863.    13.5      126295.    7
AR    11.5    124400.    5.5      125800.    19.5      125280.    27.5      125390.    8
AR    3.5     123920.    1.5      125340.                                8
AR    3.5     124780.    1.5      126210.    11.5      125100.    1.5      126524.2  9
AR    19.5    125650.    3.5      127130.    27.5      125754.                                9
AR    3.5     125330.    11.5      125540.    19.5      125940.    3.5      127410.    10
AR    3.5     125712.    1.5      127130.    5.5      125860.    19.5      126155.    11
AR    3.5     127610.                                11
AR    7.5     126000.    19.5      126300.    3.5      127760.                                12
AR    5.5     126200.    1.5      127610.    19.5      126430.    3.5      127880    13
AR    3.5     126330.    1.5      127600.    19.5      126520.    3.5      127970.    14
AR    IP      127109.9
FINISH
B      N  PRED. SUM(2J+1)  ACT. SUM(2J+1)  DIFF  MAX LEVEL  2J+1. MAX LEVEL
12.0  3      61.0      192.0      0.0      115366.9000      3.0
12.0  4      192.0      192.0      0.0      121654.0000      28.0
12.0  5      300.0      192.0      108.0      124137.0000      136.0
12.0  6      432.0      192.0      240.0      125483.0000      268.0
12.0  7      588.0      192.0      396.0      126295.0000      424.0
12.0  8      768.0      144.0      624.0      125800.0000      636.0
12.0  9      972.0      144.0      828.0      127130.0000      836.0
12.0  10     1200.0      80.0      1120.0      127410.0000      1128.0
12.0  11     1452.0      72.0      1380.0      127610.0000      1388.0
12.0  12     1728.0      64.0      1664.0      127760.0000      1672.0
12.0  13     2028.0      64.0      1964.0      127880.0000      1972.0
12.0  14     2352.0      60.0      2292.0      127970.0000      2300.0

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BAR Argon

LEAST SQUARES

T	CP/R INPUT	CP/R CALC	HH/RT INPUT	HH/RT CALC	S/R INPUT	S/R CALC	-GH/RT INPUT	-GH/RT CALC
	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION
298.15	2.5000000	2.5000000	2.5000000	2.5000000	18.6236667	18.6236667	16.1236667	16.1236667
500.00	2.5000000	2.5000000	2.5000000	2.5000000	19.9161952	19.9161952	17.4161952	17.4161952
1000.00	2.5000000	2.5000000	2.5000000	2.5000000	21.6490631	21.6490631	19.1490631	19.1490631
MAX REL ERR CP/R = 0.000000 TEMP = 1000. AVER REL ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000 MAX REL ERR HH/RT = 0.000000 TEMP = 298. AVER REL ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000 MAX REL ERR S/R = 0.000000 TEMP = 500. AVER REL ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000 MAX REL ERR GH/RT = 0.000000 TEMP = 500. AVER REL ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000 MAX ERR CP/R = 0.000000 TEMP = 1000. AVER ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000 MAX ERR HH/RT = 0.000000 TEMP = 298. AVER ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000 MAX ERR S/R = 0.000000 TEMP = 500. AVER ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000 MAX ERR GH/RT = 0.000000 TEMP = 500. AVER ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000 CP/R = 2.5000000e+00T** 0.0 (H-H0)/R CONSTANT = -0.11368684e-12, H/R CONSTANT = -0.74537500e+03, S/R CONSTANT = 0.43796749e+01								

T	CP/R INPUT	CP/R CALC	HH/RT INPUT	HH/RT CALC	S/R INPUT	S/R CALC	-GH/RT INPUT	-GH/RT CALC
	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION
1000.00	2.5000000	2.5000000	2.5000000	2.5000000	21.6490631	21.6490631	19.1490631	19.1490631
2000.00	2.5000000	2.5000000	2.5000000	2.5000000	23.3819311	23.3819311	20.8819311	20.8819311
3000.00	2.5000000	2.5000000	2.5000000	2.5000000	24.3955938	24.3955938	21.8955938	21.8955938
4000.00	2.5000000	2.5000000	2.5000000	2.5000000	25.1147990	25.1147990	22.6147990	22.6147990
5000.00	2.5000000	2.5000000	2.5000000	2.5000000	25.6726579	25.6726579	23.1726579	23.1726579
6000.00	2.5000014	2.5000006	2.5000001	2.5000000	26.1284618	26.1284618	23.6284618	23.6284618
MAX REL ERR CP/R = 0.000001 TEMP = 6000. AVER REL ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000 MAX REL ERR HH/RT = 0.000000 TEMP = 6000. AVER REL ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000 MAX REL ERR S/R = 0.000000 TEMP = 6000. AVER REL ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000 MAX REL ERR GH/RT = 0.000000 TEMP = 6000. AVER REL ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000 MAX ERR CP/R = 0.000001 TEMP = 6000. AVER ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000 MAX ERR HH/RT = 0.000000 TEMP = 6000. AVER ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000 MAX ERR S/R = 0.000000 TEMP = 6000. AVER ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000 MAX ERR GH/RT = 0.000000 TEMP = 6000. AVER ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000 CP/R = 2.5000000e+00T** 0.0 (H-H0)/R CONSTANT = -0.34106051e-12, H/R CONSTANT = -0.74537500e+03, S/R CONSTANT = 0.43796749e+01								

T	CP/R INPUT	CP/R CALC	HH/RT INPUT	HH/RT CALC	S/R INPUT	S/R CALC	-GH/RT INPUT	-GH/RT CALC
	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION	INPUT-CALC	FRACTION
6000.00	2.5000014	2.5000000	2.5000001	2.5000000	26.1284618	26.1284618	23.6284618	23.6284618
7000.00	2.5000030	2.4999969	2.5000015	2.5000000	26.5138400	26.5138400	24.0138400	24.0138400
8000.00	2.5000359	2.4999641	2.5000167	2.4998833	26.8464133	26.8464133	24.3464133	24.3464133
9000.00	2.5001650	2.4998350	2.5001131	2.4997388	27.1422446	27.1422446	24.6422446	24.6422446
10000.00	2.5007416	2.4992584	2.5004979	2.4974261	27.4024269	27.4024269	24.9024269	24.9024269
11000.00	2.5026985	2.4973015	2.5010718	2.4987833	27.6456495	27.6456495	25.1456495	25.1456495
12000.00	2.5046999	2.4953001	2.5017210	2.4980173	27.8623567	27.8623567	25.3623567	25.3623567
13000.00	2.5067532	2.4932468	2.5023601	2.4960118	28.0733960	28.0733960	25.5733960	25.5733960
14000.00	2.5088346	2.4911654	2.5030032	2.4946181	28.2722222	28.2722222	25.7722222	25.7722222
15000.00	2.5109317	2.4890683	2.5036451	2.4931315	28.4664133	28.4664133	25.9664133	25.9664133
16000.00	2.5130441	2.4869359	2.5042870	2.4916605	28.6564928	28.6564928	26.1564928	26.1564928
17000.00	2.5151650	2.4848030	2.5049289	2.4901825	28.8464133	28.8464133	26.3464133	26.3464133
18000.00	2.5172941	2.4826701	2.5055708	2.4887000	29.0364133	29.0364133	26.5364133	26.5364133
19000.00	2.5194317	2.4805372	2.5062127	2.4872188	29.2264133	29.2264133	26.7264133	26.7264133
20000.00	2.5215693	2.4784043	2.5068546	2.4857373	29.4164133	29.4164133	26.9164133	26.9164133
MAX REL ERR CP/R = 0.012343 TEMP = 19000. AVER REL ERR CP/R = 0.004478 REL LST SQ ERR CP/R = 0.005864 MAX REL ERR HH/RT = 0.018022 TEMP = 20000. AVER REL ERR HH/RT = 0.002668 REL LST SQ ERR HH/RT = 0.005166 MAX REL ERR S/R = 0.001956 TEMP = 20000. AVER REL ERR S/R = 0.000294 REL LST SQ ERR S/R = 0.000555 MAX REL ERR GH/RT = 0.000283 TEMP = 20000. AVER REL ERR GH/RT = 0.000051 REL LST SQ ERR GH/RT = 0.000084 MAX ERR CP/R = 0.052693 TEMP = 19000. AVER ERR CP/R = 0.014830 REL LST SQ ERR CP/R = 0.021188 MAX ERR HH/RT = 0.050053 TEMP = 20000. AVER ERR HH/RT = 0.007168 REL LST SQ ERR HH/RT = 0.014248 MAX ERR S/R = 0.057610 TEMP = 20000. AVER ERR S/R = 0.008506 REL LST SQ ERR S/R = 0.016311 MAX ERR GH/RT = 0.007557 TEMP = 20000. AVER ERR GH/RT = 0.001339 REL LST SQ ERR GH/RT = 0.002232 CP/R = -1.2955921e+09T** -2.0 8.2201459e+05T** -1.0 -2.0865673e+02T** 0.0 2.8064385e-02T** 1.0 -2.0298346e-06T** 2.0 (H-H0)/R CONSTANT = -0.64818047e+07, H/R CONSTANT = -0.64825501e+07, S/R CONSTANT = 0.18234371e+04								

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

Argon

NSRDS-NBS 35, 1971. Temperature cutoff 8 FILL. Expl. 1

3 L 6/88 AR	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
298.150	1000.000	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.50000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
1000.000	6000.000	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2.50000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
6000.000	20000.000	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
-1.29559206d+09	8.22014586d+05	-2.08656731d+02	2.80643848d-02	-0.02983469d-06	1.82343707d+03	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
7.52684157d-11	-1.1012887d-15	0.00000000d+00	-6.48255009d+06	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00

ORIGINAL BAR Argon

ORIGINAL		Argon						
ASSIGNED H/R AT		0 K = -745.375 K						
T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
100.00	2.50000	2.5000000	-4.9537500	15.8926004	13.3926004	20.8463504	-4.9537500	20.8463504
298.15	2.50000	2.5000000	0.0000000	18.6236667	16.1236667	18.6236667	0.0000000	18.6236667
500.00	2.50000	2.5000000	1.0092500	19.9161952	17.4161952	18.9069452	1.0092500	18.9069452
1000.00	2.50000	2.5000000	1.7546250	21.6490631	19.1490631	19.8944381	1.7546250	19.8944381
2000.00	2.50000	2.5000000	2.1273125	23.3819311	20.8819311	21.2546186	2.1273125	21.2546186
3000.00	2.50000	2.5000000	2.2515417	24.3955938	21.8955938	22.1440522	2.2515417	22.1440522
4000.00	2.50000	2.5000000	2.3136562	25.1147990	22.6147990	22.8011428	2.3136562	22.8011428
5000.00	2.50000	2.5000000	2.3509250	25.6726579	23.1726579	23.3217329	2.3509250	23.3217329
6000.00	2.50000	2.5000001	2.3757709	26.1284618	23.6284618	23.7526910	2.3757709	23.7526910
7000.00	2.50003	2.5000015	2.3935193	26.5138400	24.0138386	24.1203207	2.3935193	24.1203207
8000.00	2.50031	2.5000167	2.4068449	26.8476846	24.3476679	24.4408398	2.4068449	24.4408398
9000.00	2.50187	2.5001131	2.4172937	27.1422446	24.6421315	24.7249509	2.4172937	24.7249509
10000.00	2.50741	2.5004979	2.4259604	27.4060574	24.9055595	24.9800970	2.4259604	24.9800970
11000.00	2.52347	2.5017210	2.4339597	27.6456495	25.1439285	25.2116898	2.4339597	25.2116898
12000.00	2.55883	2.5046980	2.4425834	27.8664056	25.3617076	25.4238222	2.4425834	25.4238222
13000.00	2.62742	2.5110032	2.4536666	28.0733960	25.5623928	25.6197293	2.4536666	25.6197293
14000.00	2.75201	2.5233415	2.4701004	28.2722222	25.7488807	25.8021218	2.4701004	25.8021218
15000.00	2.91941	2.5418244	2.4921347	28.4652037	25.9235774	25.9730691	2.4921347	25.9730691
16000.00	3.18118	2.5725349	2.5259490	28.6608111	26.0882763	26.1348622	2.5259490	26.1348622
17000.00	3.52963	2.6169087	2.5730632	28.8622713	26.2453625	26.2892081	2.5730632	26.2892081
18000.00	3.81838	2.6607190	2.6193093	29.0552237	26.3945047	26.4359144	2.6193093	26.4359144
19000.00	4.26900	2.7297792	2.6905489	29.2695115	26.5397323	26.5789626	2.6905489	26.5789626
20000.00	4.48860	2.7773394	2.7400706	29.4538747	26.6765353	26.7138041	2.7400706	26.7138041

ORIGINAL		Argon						
ASSIGNED H AT		0 K = -6197.428 J/MOLE						
T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
100.00	20.78627	2078.627	-4118.800	132.139185	11135.291	17332.719	-4118.800	17332.719
298.15	20.78627	6197.428	0.000	154.846663	39970.105	46167.533	0.000	46167.533
500.00	20.78627	10393.137	4195.710	165.593404	72403.564	78600.992	4195.710	78600.992
1000.00	20.78627	20786.275	14588.847	180.001352	159215.077	165412.505	14588.847	165412.505
2000.00	20.78627	41572.550	35375.122	194.409300	347246.049	353443.477	35375.122	353443.477
3000.00	20.78627	62358.825	56161.397	202.837409	546153.402	552350.829	56161.397	552350.829
4000.00	20.78628	83145.100	76947.672	208.817248	752123.890	758321.318	76947.672	758321.318
5000.00	20.78628	103931.375	97733.947	213.455571	963346.479	969543.907	97733.947	969543.907
6000.00	20.78629	124717.653	118520.225	217.245357	1178754.491	1184951.919	118520.225	1184951.919
7000.00	20.78652	145504.010	139306.582	220.449588	1397643.106	1403840.533	139306.582	1403840.533
8000.00	20.78882	166291.314	160093.886	223.225342	1619511.425	1625708.853	160093.886	1625708.853
9000.00	20.80179	187084.942	180887.514	225.674464	1843985.237	1850182.665	180887.514	1850182.665
10000.00	20.84792	207904.148	201706.720	227.867939	2070775.239	2076972.667	201706.720	2076972.667
11000.00	20.98142	228806.429	222609.002	229.860029	22996453.893	2305851.321	222609.002	2305851.321
12000.00	21.27546	249904.040	243706.612	231.695508	2530442.054	2536639.482	243706.612	2536639.482
13000.00	21.84575	271410.893	265213.465	233.416532	2763004.017	2769201.445	265213.465	2769201.445
14000.00	22.88162	293724.870	287527.442	235.069674	2997250.569	3003447.996	287527.442	3003447.996
15000.00	24.27350	317010.610	310813.182	236.674221	3233102.708	3239300.136	310813.182	3239300.136
16000.00	26.44998	342229.873	336032.445	238.300601	3470579.741	3476777.169	336032.445	3476777.169
17000.00	29.34715	369891.357	363693.909	239.975643	3715892.025	3715892.025	363693.909	3715892.025
18000.00	31.74794	398206.348	392008.920	241.579948	3950232.712	3956430.140	392008.920	3956430.140
19000.00	35.49466	431238.748	425041.321	243.361646	4192632.525	4198829.953	425041.321	4198829.953
20000.00	37.32050	461844.323	455646.895	244.894536	4436046.393	4442243.821	455646.895	4442243.821

ORIGINAL		Argon						
ASSIGNED H AT		0 K = -1481.221 CAL/MOLE						
T DEG-K	CP CAL/MOL-K	H-H0 CAL/MOL	H-H298 CAL/MOL	S CAL/MOL-K	-(G-H0) CAL/MOL	-(G-H298) CAL/MOL	H CAL/MOL	-G CAL/MOL
100.00	4.96804	496.804	-984.417	31.582023	2661.398	4142.619	-984.417	4142.619
298.15	4.96804	1481.221	0.000	37.009241	9553.084	11034.305	0.000	11034.305
500.00	4.96804	2484.019	1002.799	39.577773	17304.867	18786.088	1002.799	18786.088
1000.00	4.96804	4968.039	3486.818	43.021356	38053.317	39534.537	3486.818	39534.537
2000.00	4.96804	9936.078	8454.857	46.464938	82993.798	84475.018	8454.857	84475.018
3000.00	4.96804	14904.117	13422.896	48.479304	130533.796	132015.017	13422.896	132015.017
4000.00	4.96804	19872.156	18390.935	49.908520	179761.924	181243.145	18390.935	181243.145
5000.00	4.96804	24840.195	23358.974	51.017106	230245.354	231726.555	23358.974	231726.555
6000.00	4.96804	29808.234	28327.014	51.922887	281729.085	283210.306	28327.014	283210.306
7000.00	4.96810	34776.293	33295.072	52.688716	334044.719	335525.940	33295.072	335525.940
8000.00	4.96865	39744.578	38263.357	53.352137	387072.520	388553.741	38263.357	388553.741
9000.00	4.97175	44714.374	43233.153	53.937491	440723.049	442204.270	43233.153	442204.270
10000.00	4.98277	49690.284	48209.063	54.461744	494927.160	496408.381	48209.063	496408.381
11000.00	5.01468	54686.049	53204.828	54.937866	549630.472	551111.692	53204.828	551111.692
12000.00	5.08496	59728.409	58247.278	55.376555	604790.166	606271.387	58247.278	606271.387
13000.00	5.22126	64868.760	63387.540	55.787890	660373.809	661855.030	63387.540	661855.030
14000.00	5.46884	70201.929	68720.708	56.183001	716360.079	717841.299	68720.708	717841.299
15000.00	5.80151	75767.354	74286.133	56.566496	772730.093	774211.314	74286.133	774211.314
16000.00	6.32170	81794.903	80313.682	56.955211	829488.466	830969.687	80313.682	830969.687
17000.00	7.01414	88406.151	86924.930	57.355555	88638.288	888119.509	86924.930	888119.509
18000.00	7.58794	95175.601	93692.381	57.738993	944128.277	945609.498	93692.381	945609.498
19000.00	8.48343	103068.535	101587.314	58.164829	1002063.223	1003544.444	101587.314	1003544.444
20000.00	8.91981	110383.442	108902.222	58.531199	1060240.534	1061721.755	108902.222	1061721.755

ORIGINAL BAR Argon

COEFFICIENTS		Argon							
ASSIGNED H/R AT		0 K = -745.375 K							
T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT	
298.15	2.50000	2.5000000	0.0000000	18.6236667	16.1236667	18.6236667	0.0000000	18.6236667	
500.00	2.50000	2.5000000	1.0092500	19.9161952	17.4161952	18.9069452	1.0092500	18.9069452	
1000.00	2.50000	2.5000000	1.7546250	21.6490631	19.1490631	19.8944381	1.7546250	19.8944381	
2000.00	2.50000	2.5000000	2.1273125	23.5819311	20.8819311	21.2546186	2.1273125	21.2546186	
3000.00	2.50000	2.5000000	2.2515417	24.3955938	21.8955938	22.1440522	2.2515417	22.1440522	
4000.00	2.50000	2.5000000	2.3136562	25.1147990	22.6147990	22.8011428	2.3136562	22.8011428	
5000.00	2.50000	2.5000000	2.3509250	25.6726579	23.1726579	23.3217329	2.3509250	23.3217329	
6000.00	2.50000	2.5000000	2.3757708	26.1284618	23.6284618	23.7526909	2.3757708	23.7526909	
7000.00	2.49494	2.5003617	2.3938796	26.5142450	24.0138833	24.1203655	2.3938796	24.1203655	
8000.00	2.48368	2.4987464	2.4055745	26.8464133	24.3676669	24.4408388	2.4055745	24.4408388	
9000.00	2.49123	2.4973788	2.4145594	27.1392646	24.6418858	24.7247052	2.4145594	24.7247052	
10000.00	2.50472	2.4974261	2.4228886	27.4024269	24.9050009	24.9795384	2.4228886	24.9795384	
11000.00	2.52103	2.4987833	2.4310219	27.6418679	25.1430845	25.2108459	2.4310219	25.2108459	
12000.00	2.55124	2.5017379	2.4396233	27.8623567	25.3606187	25.4227333	2.4396233	25.4227333	
13000.00	2.61468	2.5077049	2.4503684	28.0687779	25.5610730	25.6184095	2.4503684	25.6184095	
14000.00	2.73165	2.5191514	2.4659103	28.2664413	25.7472899	25.8005310	2.4659103	25.8005310	
15000.00	2.91719	2.5390956	2.4894039	28.4608115	25.9217159	25.9714075	2.4894039	25.9714075	
16000.00	3.17613	2.5704448	2.5238589	28.6569628	26.0865180	26.1331039	2.5238589	26.1331039	
17000.00	3.49936	2.6153123	2.5714667	28.8589372	26.2436249	26.2874705	2.5714667	26.2874705	
18000.00	3.86101	2.6745812	2.6329714	29.0690987	26.3947176	26.4361273	2.6329714	26.4361273	
19000.00	4.21631	2.7463394	2.7071091	29.2875293	26.5411899	26.5804202	2.7071091	26.5804202	
20000.00	4.49998	2.8273923	2.7901236	29.5114850	26.6840927	26.7213614	2.7901236	26.7213614	

COEFFICIENTS		Argon							
ASSIGNED H AT		0 K = -6197.428 J/MOLE							
T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL	
298.15	20.78627	6197.428	0.000	154.846663	39970.105	46167.533	0.000	46167.533	
500.00	20.78627	10393.137	4195.710	165.593404	72403.564	78600.992	4195.710	78600.992	
1000.00	20.78627	20786.275	14588.847	180.001352	159215.077	165412.505	14588.847	165412.505	
2000.00	20.78627	41572.550	35375.122	194.409300	347246.049	353443.477	35375.122	353443.477	
3000.00	20.78627	62358.825	56161.397	202.837409	546153.402	552350.829	56161.397	552350.829	
4000.00	20.78627	83145.100	76947.672	208.817248	752123.890	758321.318	76947.672	758321.318	
5000.00	20.78627	103931.375	97733.947	213.455571	963346.479	969543.907	97733.947	969543.907	
6000.00	20.78627	124717.650	118520.222	217.245357	1178754.491	1184951.919	118520.222	1184951.919	
7000.00	20.74418	145524.977	139327.549	220.452956	1397645.713	1403843.141	139327.549	1403843.141	
8000.00	20.65055	166206.813	160009.385	223.214772	1619511.362	1625708.790	160009.385	1625708.790	
9000.00	20.71339	186880.330	180682.902	225.649687	1843966.850	1850164.278	180682.902	1850164.278	
10000.00	20.82549	207648.739	201451.311	227.837753	2070728.790	2076926.218	201451.311	2076926.218	
11000.00	20.96109	228537.747	222340.319	229.828587	2299576.707	2305774.135	222340.319	2305774.135	
12000.00	21.21232	249608.700	243411.272	231.661843	2530333.416	2536530.844	243411.272	2536530.844	
13000.00	21.73978	271054.390	264856.962	233.378135	2762861.359	2769058.787	264856.962	2769058.787	
14000.00	22.71233	293237.128	287039.701	235.021609	2997065.396	3003262.823	287039.701	3003262.823	
15000.00	24.25498	316670.037	310472.609	236.637701	3232895.485	3239092.913	310472.609	3239092.913	
16000.00	26.40795	341951.827	335754.399	238.268604	3470345.830	3476543.258	335754.399	3476543.258	
17000.00	29.09550	369665.689	363468.261	239.947922	3709448.987	3715646.414	363468.261	3715646.414	
18000.00	32.10245	400251.040	394053.612	241.695312	3950264.576	3956462.004	394053.612	3956462.004	
19000.00	35.05655	433854.863	427657.435	243.511455	4192862.790	4199060.218	427657.435	4199060.218	
20000.00	37.41512	470167.636	463970.208	245.373537	4437303.106	4443500.534	463970.208	4443500.534	

COEFFICIENTS		Argon							
ASSIGNED H AT		0 K = -1481.221 CAL/MOLE							
T DEG-K	CP CAL/MOL-K	H-H0 CAL/MOL	H-H298 CAL/MOL	S CAL/MOL-K	-(G-H0) CAL/MOL	-(G-H298) CAL/MOL	H CAL/MOL	-G CAL/MOL	
298.15	4.96804	1481.221	0.000	37.009241	9553.084	11034.305	0.000	11034.305	
500.00	4.96804	2484.019	1002.799	39.577773	17304.867	18786.088	1002.799	18786.088	
1000.00	4.96804	4968.039	3486.818	43.021356	38053.317	39534.537	3486.818	39534.537	
2000.00	4.96804	9936.078	8454.857	46.464938	82993.798	84475.018	8454.857	84475.018	
3000.00	4.96804	14904.117	13422.896	48.479304	130533.796	132015.017	13422.896	132015.017	
4000.00	4.96804	19872.156	18390.935	49.908520	179761.924	181243.145	18390.935	181243.145	
5000.00	4.96804	24840.195	23358.974	51.017106	230245.334	231726.555	23358.974	231726.555	
6000.00	4.96804	29808.234	28327.013	51.922886	281729.085	283210.306	28327.013	283210.306	
7000.00	4.95798	34781.304	33300.083	52.689521	334045.342	335526.563	33300.083	335526.563	
8000.00	4.93560	39724.382	38243.161	53.349611	387072.505	388553.726	38243.161	388553.726	
9000.00	4.95062	44665.471	43184.250	53.931569	440718.654	442199.875	43184.250	442199.875	
10000.00	4.97741	49629.240	48148.019	54.454530	494916.059	496397.280	48148.019	496397.280	
11000.00	5.00982	54621.832	53140.612	54.930351	549612.024	551093.244	53140.612	551093.244	
12000.00	5.06987	59657.911	58176.690	55.368509	604764.201	606245.422	58176.690	606245.422	
13000.00	5.19593	64783.554	63302.333	55.778713	660379.713	661820.934	63302.333	661820.934	
14000.00	5.42838	70085.356	68604.135	56.171513	716315.821	717797.042	68604.135	717797.042	
15000.00	5.79708	75685.955	74204.734	56.557768	772680.565	774161.786	74204.734	774161.786	
16000.00	6.31165	81728.448	80247.227	56.947563	829432.560	830913.781	80247.227	830913.781	
17000.00	6.95399	88352.220	86870.999	57.348930	886579.586	888060.807	86870.999	888060.807	
18000.00	7.67267	95662.295	94181.074	57.766566	944135.893	945617.114	94181.074	945617.114	
19000.00	8.37872	103693.801	102212.580	58.200635	1002118.258	1003599.479	102212.580	1003599.479	
20000.00	8.94243	112372.762	110891.541	58.645683	1060540.895	1062022.116	110891.541	1062022.116	

COEFFICIENTS BAR Argon

Example 2 (C₂H₃(g) by Method ADD with Wilhoit Extrapolation)

Problem.—Estimate thermodynamic properties for the C₂H₃ radical by adding group properties using method ADD and then extrapolate these properties to higher temperatures by means of the Wilhoit fit. Finally, obtain a least-squares fit of the previously generated data. C₂H₃ can be represented as

being formed from two CDH2 groups $\begin{pmatrix} \text{H} \\ | \\ \text{H}-\text{C}=\end{pmatrix}$ with a hydrogen atom removed by subtracting an HVIN group (See table IX). Inasmuch as the group data extend to only 3000 K, extrapolation to higher temperatures, e.g., to 5000 K, can be accomplished by means of the Wilhoit fit.

The input data set for example 2 consists of 12 records. The first is a NAME record giving the species name and comments. The second is a formula record. It gives a formula only. With method ADD, the heat of formation comes from the group additivity calculation and any value on the formula record is ignored. The DATE record gives a code (G 3/91) to represent Group additivity, March 1991. The OUTP record calls for a many-figured table (MFIG) in SI units (JOULES) and least-squares coefficients (LSQS). There are also two LSTS records giving five EXP values (q_i in eq. (11)) for the first temperature interval (1 in column 80), namely the default interval 298.15 to 1000 K. These are the same exponents as in the equation representing the group data (see table X). Since no information is given for the second interval, it will be the

default interval of 1000 to 6000 K and the default equation for C_p^o with q_i values in equation (17).

There are two METH records each preceded by a set of corresponding TEMP records. For METH ADD, the temperature schedule is 298.15 K and 300 to 3000 K in 100-degree increments. For METH WILH, the schedule is 3500 to 6000 K in 500-degree increments. METH ADD is followed by one data record and METH WILH is the only method with no data records. The data record following the METH ADD record has a blank record ID. The labels on this record contain the group names, left-adjusted, followed by the number of times the group should be added or subtracted as well as the symmetry number (SYMNO) and statistical weight (STATWT) of the species formed. In this case all the numerical values are integers which should always be followed by a decimal. Numerical values should never encroach on the label spaces. The last record is the required FINISH record.

The first part of the output consists of input record images and some additional intermediate information. The molecular weight is inserted after the METH ADD record and the Wilhoit coefficients and integration constants are inserted after the METH WILH record image. The least-squares output is detailed in the section **Tables of least-squares errors**. The output table in SI units is described in appendix C in the section **Tables of original thermodynamic properties**. The columns for H-H0 and -(G-H0) are blank because no $H_{298.15}^o - H_0^o$ value (H298H0) was available.

Input. - The input data set for C₂H₃, example 2, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a NAME	C2H3	RADICAL	GROUP	ADDITION WITH WILHOIT	EXTRAPOLATION.			Expl.	2
C2H3									
DATE	G 3/91								
TEMP	T	298.15	T	300.	I	100.	T	3000.	
OUTP	MFIG		JOULES		LSQS				
LSTS	EXP	0.	EXP	1.	EXP	2.	EXP	3.	1
LSTS	EXP	4.							1
METH	ADD								
	CDH2	2.	HVIN	-1.	SYMNO	1.	STATWT	2.	
TEMP	T	3500.	I	500.	T	6000.			
METH	WILH								
FINISH									

^aAll alphanumeric characters.

Listed output. - The listed output for C₂H₃, example 2, is as follows:

```

NAME C2H3 RADICAL      GROUP ADDITION WITH WILHOIT EXTRAPOLATION.      Exp1. 2
C2H3
DATE G 3/91
OUTP MFIG              JOULES              LSQS
LSTS EXP      0.      EXP      1.      EXP      2.      EXP      3.      1
LSTS EXP      4.              1
TEMP T      298.15      T      300.      I      100.      T      5000.
METH ADD
MOLECULAR WT. = 27.04582
      CDH2      2.000000HVIN      -1.000000SYMNO      1.000000STATHT      2.000000
TEMP T      3500.      I      500.      T      6000.
METH WILH
      WILHOIT COEFFICIENTS
      A(0) = 0.924838250e+02      A(1) = -0.367448984e+03      A(2) = 0.498539437e+03      A(3) = -0.225971567e+03
INTEGRATION CONSTANTS:      H/R = 0.788004609e+05      S/R = -0.172647715e+02
B = 150.0      CPO/R = 4.0000      CPI/R = 15.0000      NON-LINEAR      NO. ATOMS = 5
FINISH

LEAST SQUARES

      T      CP/R INPUT      CP/R CALC      HH/RT INPUT      HH/RT CALC      S/R INPUT      S/R CALC      -GH/RT INPUT      -GH/RT CALC
      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION
298.15      5.1334587      5.1334587      0.0000000      0.0000000      28.1531124      28.1531124      28.1531124      28.1531124
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
300.00      5.1531178      5.1531178      0.0317170      0.0317170      28.1849275      28.1849275      28.1532105      28.1532105
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
400.00      6.1157304      6.1157304      1.4362780      1.4362780      29.8036844      29.8036844      28.3674064      28.3674064
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
500.00      6.9177687      6.9177687      2.4546466      2.4546466      31.2570661      31.2570661      28.8024195      28.8024195
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
600.00      7.6026413      7.6026413      3.2569567      3.2569567      32.5803752      32.5803752      29.3234185      29.3234185
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
700.00      8.2006088      8.2006088      3.9213848      3.9213848      33.7982078      33.7982078      29.8768250      29.8768250
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
800.00      8.7287846      8.7287846      4.4899800      4.4899800      34.9284535      34.9284535      30.4334733      30.4334733
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
900.00      9.1911343      9.1911343      4.9872741      4.9872741      35.9839172      35.9839172      30.9966431      30.9966431
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
1000.00      9.5784758      9.5784758      5.4277252      5.4277252      36.9730816      36.9730816      31.5453565      31.5453565
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
MAX REL ERR CP/R = 0.000000      TEMP = 400.      AVER REL ERR CP/R = 0.000000      REL LST SQ ERR CP/R = 0.000000
MAX REL ERR HH/RT = 0.000000      TEMP = 400.      AVER REL ERR HH/RT = 0.000000      REL LST SQ ERR HH/RT = 0.000000
MAX REL ERR S/R = 0.000000      TEMP = 500.      AVER REL ERR S/R = 0.000000      REL LST SQ ERR S/R = 0.000000
MAX REL ERR GH/RT = 0.000000      TEMP = 700.      AVER REL ERR GH/RT = 0.000000      REL LST SQ ERR GH/RT = 0.000000
MAX REL CP/R = 0.000000      TEMP = 900.      AVER REL CP/R = 0.000000      LST SQ ERR CP/R = 0.000000
MAX REL HH/RT = 0.000000      TEMP = 500.      AVER REL HH/RT = 0.000000      LST SQ ERR HH/RT = 0.000000
MAX REL S/R = 0.000000      TEMP = 500.      AVER REL S/R = 0.000000      LST SQ ERR S/R = 0.000000
MAX REL GH/RT = 0.000000      TEMP = 700.      AVER REL GH/RT = 0.000000      LST SQ ERR GH/RT = 0.000000
CP/R = 6.7053736e-011** 0.0      2.0520078e-021** 1.0      -2.3229402e-051** 2.0      1.7095426e-081** 3.0      -5.4781628e-121** 4.0
(H-H0)/R CONSTANT = -0.9379408e+03, H/R CONSTANT = 0.80540638e+05, S/R CONSTANT = 0.19106863e+02

      T      CP/R INPUT      CP/R CALC      HH/RT INPUT      HH/RT CALC      S/R INPUT      S/R CALC      -GH/RT INPUT      -GH/RT CALC
      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION      INPUT-CALC      FRACTION
1000.00      9.5784758      9.5784758      5.4277252      5.4277252      36.9730816      36.9730816      31.5453565      31.5453565
0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
1100.00      9.9445347      9.9445347      5.8221381      5.8221381      37.9036300      37.9036300      32.0814919      32.0814919
-0.0031261      -0.0031261      -0.0001256      -0.0001256      -0.0001285      -0.0001285      -0.0000054      -0.0000054
1200.00      10.2624975      10.2624975      6.1792256      6.1792256      38.7828698      38.7828698      32.6036422      32.6036422
-0.0032441      -0.0032441      -0.0004027      -0.0004027      -0.0004287      -0.0004287      -0.0000111      -0.0000111
1300.00      10.5390577      10.5390577      6.5042090      6.5042090      39.6154873      39.6154873      33.1112782      33.1112782
-0.0011634      -0.0011634      -0.0005493      -0.0005493      -0.0006147      -0.0006147      -0.0000155      -0.0000155
1400.00      10.7792887      10.7792887      6.8011941      6.8011941      40.4051653      40.4051653      33.6043224      33.6043224
-0.0014425      -0.0014425      -0.0004994      -0.0004994      -0.0006047      -0.0006047      -0.0000150      -0.0000150
1500.00      10.9878845      10.9878845      7.0735169      7.0735169      41.1564927      41.1564927      34.0829758      34.0829758
0.0034784      0.0034784      -0.0002968      -0.0002968      -0.0004204      -0.0004204      -0.0001055      -0.0001055
1600.00      11.1691592      11.1691592      7.3239872      7.3239872      41.8711722      41.8711722      34.5475958      34.5475958
0.0043931      0.0043931      -0.0000258      -0.0000258      -0.0001700      -0.0001700      -0.0000041      -0.0000041
1700.00      11.3270474      11.3270474      7.5546885      7.5546885      42.5535297      42.5535297      34.9866308      34.9866308
0.0040681      0.0040681      0.0002304      0.0002304      0.0000926      0.0000926      -0.0001578      -0.0001578
1800.00      11.4651042      11.4651042      7.7683818      7.7683818      43.2049603      43.2049603      35.4365785      35.4365785
0.0026928      0.0026928      0.0004095      0.0004095      0.0002904      0.0002904      -0.0001191      -0.0001191
1900.00      11.5865047      11.5865047      7.9662075      7.9662075      43.8281674      43.8281674      35.8619599      35.8619599
0.0006474      0.0006474      0.0000559      0.0000559      0.0000887      0.0000887      -0.0000946      -0.0000946
2000.00      11.6940448      11.6940448      8.1499633      8.1499633      44.4252656      44.4252656      36.2753024      36.2753024
-0.0015973      -0.0015973      0.0004300      0.0004300      0.0003591      0.0003591      -0.0000081      -0.0000081
2100.00      11.7901404      11.7901404      8.3210581      8.3210581      44.9981873      44.9981873      36.6771292      36.6771292
-0.0035658      -0.0035658      0.0003023      0.0003023      0.0002316      0.0002316      -0.0000053      -0.0000053
2200.00      11.8748279      11.8748279      8.4806686      8.4806686      45.5486655      45.5486655      37.0679520      37.0679520
-0.0048367      -0.0048367      0.0000775      0.0000775      0.0000331      0.0000331      -0.0000044      -0.0000044
2300.00      11.9557641      11.9557641      8.6301433      8.6301433      46.0784120      46.0784120      37.4483145      37.4483145
-0.0051185      -0.0051185      -0.0001463      -0.0001463      -0.0001922      -0.0001922      -0.0000042      -0.0000042
2400.00      12.0282262      12.0282262      8.7702412      8.7702412      46.5887969      46.5887969      37.8185557      37.8185557
0.0046624      0.0046624      -0.0003555      -0.0003555      -0.0003962      -0.0003962      -0.0000085      -0.0000085
2500.00      12.0951116      12.0951116      8.9019158      8.9019158      47.0811868      47.0811868      38.1792170      38.1792170
-0.0023753      -0.0023753      -0.0001964      -0.0001964      0.0000535      0.0000535      -0.0000731      -0.0000731
2600.00      12.1569382      12.1569382      9.0253358      9.0253358      47.5567863      47.5567863      38.5308506      38.5308506
0.0002843      0.0002843      0.0000234      0.0000234      0.0000122      0.0000122      -0.0000921      -0.0000921
2700.00      12.2138462      12.2138462      9.1429680      9.1429680      48.0166759      48.0166759      38.8737679      38.8737679
0.0031490      0.0031490      -0.0002578      -0.0002578      -0.0000136      -0.0000136      -0.0001092      -0.0001092
2800.00      12.2655882      12.2655882      9.2535822      9.2535822      48.4618162      48.4618162      39.2082340      39.2082340
0.0053888      0.0053888      -0.0002342      -0.0002342      -0.0003552      -0.0003552      -0.0001210      -0.0001210
2900.00      12.3115491      12.3115491      9.3582548      9.3582548      48.8930517      48.8930517      39.5349770      39.5349770
0.0058806      0.0058806      0.0004777      0.0004777      -0.0001505      -0.0001505      -0.0001256      -0.0001256
3000.00      12.3507263      12.3507263      9.4573714      9.4573714      49.3111136      49.3111136      39.8537422      39.8537422
0.0031944      0.0031944      0.0001333      0.0001333      0.0000149      0.0000149      -0.0001234      -0.0001234

ORIGINAL      BAR      C2H3 RADICAL

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3500.00	12.5136171	12.5139980	9.8830643	9.8827806	51.2279962	51.2277975	41.3449320	41.3450169
	-0.0003809	-0.0000304	0.0002836	0.0000287	0.0001987	0.0000039	-0.0000849	-0.0000021
4000.00	12.6258090	12.6286924	10.2193107	10.2192865	52.9067248	52.9067615	42.6874141	42.6874750
	-0.0028834	-0.0002284	0.0000242	0.0000024	-0.0000368	-0.0000007	-0.0000609	-0.0000014
4500.00	12.7057216	12.7082897	10.4913770	10.4916897	54.3986970	54.3990884	43.9073201	43.9073987
	-0.0025681	-0.0002021	-0.0003127	-0.0000298	-0.0003914	-0.0000072	-0.0000787	-0.0000018
5000.00	12.7644316	12.7638239	10.7158907	10.7162859	55.7405685	55.7410827	45.0246778	45.0247968
	0.0006078	0.0000476	-0.0003952	-0.0000369	-0.0005142	-0.0000092	-0.0001190	-0.0000026
5500.00	12.8086825	12.8053269	10.9042239	10.9043782	56.9593193	56.9596208	46.0550954	46.0552426
	0.0033555	0.0002620	-0.0001544	-0.0000142	-0.0003015	-0.0000053	-0.0001472	-0.0000032
6000.00	12.8427587	12.8442720	11.0644080	11.0643857	58.0753434	58.0754710	47.0109354	47.0110853
	-0.0015133	-0.0001178	0.0000223	0.0000020	-0.0001276	-0.0000022	-0.0001499	-0.0000032
MAX REL ERR CP/R	= 0.000478	TEMP = 2900.	AVER REL ERR CP/R	= 0.000237	REL LST SQ ERR CP/R	= 0.000274		
MAX REL ERR HH/RT	= 0.000084	TEMP = 1300.	AVER REL ERR HH/RT	= 0.000033	REL LST SQ ERR HH/RT	= 0.000040		
MAX REL ERR S/R	= 0.000016	TEMP = 1300.	AVER REL ERR S/R	= 0.000007	REL LST SQ ERR S/R	= 0.000008		
MAX REL ERR GH/RT	= 0.000004	TEMP = 1600.	AVER REL ERR GH/RT	= 0.000002	REL LST SQ ERR GH/RT	= 0.000003		
MAX REL CP/R	= 0.005881	TEMP = 2900.	AVER REL CP/R	= 0.002786	LST SQ ERR CP/R	= 0.003226		
MAX REL HH/RT	= 0.000549	TEMP = 1300.	AVER REL HH/RT	= 0.000268	LST SQ ERR HH/RT	= 0.000318		
MAX REL S/R	= 0.000615	TEMP = 1300.	AVER REL S/R	= 0.000299	LST SQ ERR S/R	= 0.000354		
MAX REL GH/RT	= 0.000150	TEMP = 6000.	AVER REL GH/RT	= 0.000088	LST SQ ERR GH/RT	= 0.000098		

CP/R = 2.0575702e+06T** -2.0 -9.4600005e+03T** -1.0 1.8762547e+01T** 0.0 -2.2520423e-03T** 1.0 5.3448381e-07T** 2.0
 -6.7520919e-11T** 3.0 3.4387285e-15T** 4.0
 (H-H0)/R CONSTANT = 0.55034170e+05, H/R CONSTANT = 0.13651275e+06, S/R CONSTANT = -0.99058768e+02

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

C2H3 RADICAL GROUP ADDITION WITH WILHOIT EXTRAPOLATION. Expt. 2

2 G 3/91 C	2.00H	3.00	0.00	0.00	0.00	0.00	27.04582	677454.462
298.150	1000.000	5.00	1.00	2.00	3.00	4.00	0.00	0.000
6.70537360d-01	2.05200777d-02	-2.32294021d-05	1.70954257d-08	-5.47816280d-12	0.00000000d+00	0.00000000d+00	8.05406384d+04	1.91068625d+01
1000.000	6000.000	7.00	-2.00	-1.00	0.00	1.00	2.00	3.00
2.05757019d+06	-9.46000054d+03	1.87625468d+01	-2.25204228d-03	5.34483811d-07	-6.75209185d-11	3.43872846d-15	0.00000000d+00	1.36512749d+05
								-9.90587681d+01

ORIGINAL C2H3 RADICAL

ASSIGNED H AT 298 K = 677454.462 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
298.15	42.68219		0.000	234.079335		69790.754	677454.462	-607663.708
300.00	42.84565		79.115	234.343862		70224.045	677533.575	-607230.417
400.00	50.84930		4776.779	247.803032		94344.434	682231.241	-583110.028
500.00	57.51786		10204.592	259.887189		119739.002	687659.054	-557715.459
600.00	65.21224		16247.999	270.889856		146285.914	693702.461	-531168.548
700.00	68.18404		22823.075	281.015536		173887.801	700277.537	-503566.661
800.00	72.57557		29865.587	290.412974		202464.793	707320.049	-474989.649
900.00	76.41978		37520.066	299.188639		231949.709	714774.528	-445504.753
1000.00	79.64033		45128.875	307.413057		262284.182	722583.337	-415170.230
1100.00	82.68393		53249.048	315.150111		293416.074	730703.510	-384038.338
1200.00	85.32764		61652.679	322.460558		325299.991	739107.141	-352154.471
1300.00	87.62710		70303.105	329.383365		357895.270	747757.566	-319559.192
1400.00	89.62450		79168.034	335.952071		391164.865	756622.496	-286289.537
1500.00	91.35888		88219.241	342.196070		425074.864	765673.703	-252379.537
1600.00	92.86609		97432.241	348.141481		459594.129	774886.703	-217860.333
1700.00	94.17885		106785.980	353.811748		494693.992	784240.442	-182760.470
1800.00	95.32672		116262.518	359.228074		530348.016	793716.980	-147106.446
1900.00	96.33611		125846.712	364.409736		566531.786	803301.174	-110922.676
2000.00	97.23025		135525.902	369.374315		603222.729	812980.364	-74231.733
2100.00	98.02924		145289.594	374.137878		640399.950	822744.056	-37054.512
2200.00	98.75000		155129.146	378.715109		678044.095	832583.608	589.633
2300.00	99.40632		165037.450	383.119417		716137.209	842491.912	38682.748
2400.00	100.00881		175008.619	387.363017		754662.623	852463.081	77208.161
2500.00	100.56493		185037.670	391.456999		793604.827	862492.132	116150.365
2600.00	101.07898		195120.206	395.411375		832949.370	872574.668	155494.908
2700.00	101.55213		205252.106	399.235132		872682.749	882706.568	195228.237
2800.00	101.98236		215429.205	402.936255		912792.310	892883.667	235337.848
2900.00	102.36450		225646.978	406.521767		953266.147	903101.440	275811.636
3000.00	102.69024		235900.228	409.997747		994093.013	913354.690	316638.551
3500.00	104.04459		287604.928	425.935687		1203169.977	965059.390	525715.515
4000.00	104.97742		339874.244	439.893492		1419699.725	1017328.706	742245.263
4500.00	105.64185		392537.964	452.298511		1642805.334	1069992.426	963550.872
5000.00	106.12999		445486.902	463.455514		1871790.669	1122941.364	1194336.208
5500.00	106.49792		498648.031	473.588830		2106090.531	1176102.493	1428636.070
6000.00	106.78125		551970.787	482.868024		2345237.356	1229425.249	1667782.894

ORIGINAL BAR C2H3 RADICAL

Example 3 (C₄H₄(g) by Method READIN with Wilhoit Extrapolation)

Problem.—Use method READIN to process thermodynamic data obtained from the literature. Inasmuch as the data to be processed are available to only 1500 K, use the Wilhoit fit to extrapolate to higher temperatures.

The input follows the same pattern as in the first two examples. The NAME record gives the name and reference for the species. The second record, the required formula record, gives the formula and heat of formation at 298.15 K (HF298)—namely, 435 000 J/mol. This is followed by a DATE record where X10/85 was chosen to represent the Texas TRC Thermodynamic Tables along with the date of the particular table. The two REFN records give more information on the reference. The first label ATM on the OUP record specifies that the pressure unit in the output entropy and Gibbs energy functions be in atmospheres rather than the default unit which is bars. The remaining OUP record labels call for many figures tables (MFIG), in both dimensionless (DMLESS) and joules (JOULES) energy units.

There are two METH records. The first is a READIN method with no preceding TEMP records since the temper-

atures for the data come from the data records. The METH WILH record is for Wilhoit extrapolation and the TEMP record which precedes it gives the extrapolation schedule. The KJOULE label on the METH READIN record specifies that the input enthalpy values are in units of kJ/mol. However, C_p^o and S_T^o values are in J/mol-K whether the label is KJOULE or JOULES. The BAR label specifies that the standard state pressure in the entropy values on the data records is one bar. The 19 data records have the optional record ID of C4H4. The METH WILH record has no other labels since the molecule is nonlinear, the default structure. Linear molecules require a LINE label. Since this method has no data records, it is followed by the final FINISH record.

The listed output consists of the input record images, the Wilhoit coefficients and integration constants, and the two tables requested on the OUP record. It should be noted that the OUP record specifies one atmosphere (ATM) for the output standard state entropy pressure while the METH record indicates the standard state pressure is one bar (BAR) for the input entropy. Thus, at T = 298.15 K, S_T^o = 251.67 J/mol-K in the input and S_T^o = 251.56 J/mol-K in the output.

Input. - The input data set for C₄H₄, example 3, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	CYCLOBUTADIENE	TRC TABLES T,U,V,W	-2920, 435000.	JOULES	OCT 31, 1985.		Expl.	3
a	DATE	X10/85	HF298						
a	REFN	TRC THERMODYNAMIC	TABLES - HYDROCARBONS.						
a	REFN	College Station, TX 77843-3111.	Tables			The Texas A&M University System,			
	OUTP	ATM	DMLESS	t,u,v,w-2920, Oct. 31, 1985.	MFIG				
	METH	READIN	KJOULE		BAR	JOULES			
	C4H4	T	CP	33.2600	H-HO	0.166300D 01S		182.78000	
	C4H4	T	CP	33.6300	H-HO	0.333000D 01S		205.88000	
	C4H4	T	CP	36.6100	H-HO	0.507100D 01S		219.96000	
	C4H4	T	CP	43.0200	H-HO	0.705000D 01S		231.30000	
	C4H4	T	CP	55.9800	H-HO	0.106550D 02S		246.56000	
	C4H4	T	CP	60.7500	H-HO	0.121140D 02S		251.67000	
	C4H4	T	CP	61.1000	H-HO	0.122270D 02S		252.04000	
	C4H4	T	CP	79.3000	H-HO	0.192670D 02S		272.17000	
	C4H4	T	CP	94.4500	H-HO	0.279830D 02S		291.56000	
	C4H4	T	CP	106.5000	H-HO	0.380530D 02S		309.88000	
	C4H4	T	CP	116.1700	H-HO	0.492040D 02S		327.05000	
	C4H4	T	CP	124.1200	H-HO	0.612310D 02S		343.10000	
	C4H4	T	CP	130.8100	H-HO	0.739900D 02S		358.12000	
	C4H4	T	CP	136.5000	H-HO	0.873600D 02S		372.20000	
	C4H4	T	CP	141.5000	H-HO	0.101260D 03S		385.50000	
	C4H4	T	CP	145.7000	H-HO	0.115630D 03S		398.00000	
	C4H4	T	CP	149.4000	H-HO	0.130390D 03S		409.80000	
	C4H4	T	CP	152.7000	H-HO	0.145500D 03S		421.00000	
	C4H4	T	CP	155.5000	H-HO	0.160920D 03S		431.60000	
	TEMP	T		200.	T	5000.			
	METH	WILH	I						
	FINISH								

*All alphanumeric characters.

Listed output. - The listed output for C₄H₄, example 3, is as follows:

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NAME  CYCLOBUTADIENE      TRC TABLES T,U,V,W-2920, OCT 31, 1985.          Expl. 3
C4H4      HF298      435000.      JOULES
DATE  X10/85
REFN  TRC THERMODYNAMIC TABLES - HYDROCARBONS.  The Texas A&M University System,
REFN  College Station, TX 77843-3111.  Tables t,u,v,w-2920, Oct.31,1985.
OUP  ATM          DMLESS          MFIG          JOULES
METH READIN          KJOULE          BAR
C4H4  T          50.000  CP          33.2600  H-H0  0.166300D 01S          182.78000
C4H4  T          100.000 CP          33.6300  H-H0  0.333000D 01S          205.88000
C4H4  T          150.000 CP          36.6100  H-H0  0.507100D 01S          219.96000
C4H4  T          200.000 CP          43.0200  H-H0  0.705000D 01S          231.30000
C4H4  T          273.160 CP          55.9800  H-H0  0.106550D 02S          246.56000
C4H4  T          298.150 CP          60.7500  H-H0  0.121140D 02S          251.67000
C4H4  T          300.000 CP          61.1000  H-H0  0.122270D 02S          252.04000
C4H4  T          400.000 CP          79.3000  H-H0  0.192670D 02S          272.17000
C4H4  T          500.000 CP          94.4500  H-H0  0.279830D 02S          291.56000
C4H4  T          600.000 CP          106.5000 H-H0  0.380530D 02S          309.88000
C4H4  T          700.000 CP          116.1700 H-H0  0.492040D 02S          327.05000
C4H4  T          800.000 CP          124.1200 H-H0  0.612310D 02S          343.10000
C4H4  T          900.000 CP          130.8100 H-H0  0.739900D 02S          358.12000
C4H4  T          1000.000 CP          136.5000 H-H0  0.873600D 02S          372.20000
C4H4  T          1100.000 CP          141.5000 H-H0  0.101260D 03S          385.50000
C4H4  T          1200.000 CP          145.7000 H-H0  0.115630D 03S          398.00000
C4H4  T          1300.000 CP          149.4000 H-H0  0.130390D 03S          409.80000
C4H4  T          1400.000 CP          152.7000 H-H0  0.145500D 03S          421.00000
C4H4  T          1500.000 CP          155.5000 H-H0  0.160920D 03S          431.60000
                                ATM      CYCLOBUTADIENE

TEMP  T          1600.      I          200.      T          5000.
METH  WILH
      WILHOIT COEFFICIENTS
      A(0) = 0.415261964e+00      A(1) = 0.540942637e+01      A(2)          = -0.610546449e+01      A(3) = -0.117525765e+01
INTEGRATION CONSTANTS:      H/R = 0.103765248e+05      S/R = -0.890756216e+02
B = 200.0      CP0/R = 4.0000      CPI/R = 22.0000      NON-LINEAR      NO. ATOMS = 8
FINISH

                                ORIGINAL          ATM      CYCLOBUTADIENE

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ORIGINAL CYCLOBUTADIENE
ASSIGNED H/R AT 0 K = 50861.205 K

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
50.00	4.00024	4.0002357	-25.1391844	21.9700928	17.9698570	47.1092772	1021.2243415	-999.2542488
100.00	4.04474	4.0050466	-10.5646635	24.7483683	20.7433217	35.3130318	512.6170995	-487.8687312
150.00	4.40315	4.0659842	-5.6471558	26.4417935	22.3758092	32.0889493	343.1406862	-316.6988927
200.00	5.17409	4.2395764	-3.0452787	27.8056742	23.5660978	30.8509529	258.5456028	-230.7399236
273.16	6.73281	4.6913700	-0.6423941	29.6410199	24.9496498	30.2834139	190.8870257	-161.2460058
298.15	7.30650	4.8867047	0.0000000	30.2556081	25.3689034	30.2556081	175.4760231	-145.2204150
300.00	7.34860	4.9018723	0.0453023	30.3001086	25.3982363	30.2548063	174.4392233	-144.1391147
400.00	9.53754	5.7931856	2.1507581	32.7211773	26.9279917	30.5704192	132.9661989	-100.2250215
500.00	11.35966	6.7311243	3.8171823	35.0532450	28.3221207	31.2360628	108.4535348	-73.4002898
600.00	12.80893	7.6278297	5.1995447	37.2566220	29.6287922	32.0570773	92.3965052	-55.1398832
700.00	13.97196	8.4540675	6.3726803	39.3216866	30.8676191	32.9490062	81.1129322	-41.7912456
800.00	14.92812	9.2054433	7.3842295	41.2520469	32.0466036	33.8678174	72.7819499	-31.5299030
900.00	15.73274	9.8876676	8.2688109	43.0585273	33.1708597	34.7897164	66.4001179	-23.5415906
1000.00	16.41708	10.5069331	9.0499621	44.7519524	34.2450194	35.7019904	61.3681384	-16.6161859
1100.00	17.01844	11.0715539	9.7470348	46.3515656	35.2800118	36.6049264	57.3090132	-10.9574476
1200.00	17.52358	11.5891776	10.3750351	47.8549615	36.2657839	37.4799264	53.9735154	-6.1185539
1300.00	17.96859	12.0632485	10.9425015	49.2741672	37.2109188	38.3316657	51.1872525	-1.9130853
1400.00	18.36548	12.4996628	11.4589692	50.6212099	38.1215471	39.1622407	48.8290952	1.7921148
1500.00	18.70224	12.9027447	11.9314307	51.8960896	38.9933649	39.9646389	46.8102149	5.0858747
1600.00	18.99517	13.2691069	12.3585000	53.1070325	39.8379256	40.7485325	45.0573602	8.0496723
1800.00	19.33589	13.9197380	13.1103097	55.3509888	41.4393608	42.2487891	42.1759632	13.1831356
2000.00	19.68191	14.4793212	13.7508357	57.4149494	42.9356282	43.6411137	39.9099238	17.5050256
2200.00	19.95893	14.9653234	14.3030638	59.3042970	44.3389736	45.0012332	38.0840530	21.2202440
2400.00	20.18447	15.3911641	14.7840929	61.0509441	45.6597799	46.2668312	36.5833330	24.4676111
2600.00	20.37080	15.7672659	15.2068925	62.6741498	46.9068838	47.4672573	35.3226880	27.3448818
2800.00	20.52673	16.1018181	15.5814713	64.1896603	48.0878422	48.6081890	34.2665343	29.9231260
3000.00	20.65870	16.4013296	15.9156726	65.6104809	49.2091514	49.6948084	33.3550647	32.2554163
3200.00	20.77154	16.6710308	16.2157274	66.9474573	50.2764264	50.7317299	32.5651575	34.5822998
3400.00	20.86888	16.9151685	16.4866476	68.2097152	51.2945467	51.7237676	31.8743465	36.3353637
3600.00	20.95353	17.1372236	16.7325095	69.4049981	52.2677745	52.6724887	31.2653362	38.1396619
3800.00	21.02769	17.3400752	16.9566618	70.5399269	53.1998517	53.5832651	30.7246029	39.8153240
4000.00	21.09308	17.5261239	17.1618812	71.6202032	54.0940793	54.4581220	30.2414252	41.3787780
4200.00	21.15109	17.6973870	17.3504892	72.6507692	54.9533822	55.3002801	29.8071978	42.8455714
4400.00	21.20284	17.8555715	17.5244417	73.6359350	55.7803635	56.1114933	29.4149364	44.2209986
4600.00	21.24923	18.0021314	17.6853986	74.5794805	56.5773490	56.8940819	29.0589152	45.5205653
4800.00	21.29102	18.1383128	17.8347772	75.4847378	57.3464250	57.6499606	28.7343973	46.7503405
5000.00	21.32882	18.2651896	17.9737954	76.3546587	58.0894691	58.3808633	28.4374306	47.9172281

ORIGINAL ATM CYCLOBUTADIENE

ORIGINAL CYCLOBUTADIENE
ASSIGNED H AT 0 K = 422886.000 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
50.00	33.26000	1663.000	-10451.000	182.670556	7470.528	19584.528	424549.000	-415415.472
100.00	33.63000	3330.000	-8784.000	205.770556	17247.056	29361.056	426216.000	-405638.944
150.00	36.61000	5071.000	-7043.000	219.850556	27906.583	40020.583	427957.000	-394979.417
200.00	43.02000	7050.000	-5064.000	231.190556	39188.111	51302.111	429936.000	-383697.839
273.16	55.98000	10655.000	-1459.000	246.450556	56665.434	68779.434	433541.000	-366220.566
298.15	60.75000	12114.000	0.000	251.560556	62888.780	75002.780	435000.000	-359997.220
300.00	61.10000	12227.000	113.000	251.930556	63352.167	75466.167	435113.000	-359533.833
400.00	79.30000	19267.000	7153.000	272.060556	89557.222	101671.222	442153.000	-333328.778
500.00	94.45000	27883.000	15849.000	291.450556	117742.278	129856.278	450869.000	-305143.722
600.00	106.50000	38053.000	25939.000	309.770556	147809.334	159923.334	460939.000	-275076.666
700.00	116.17000	49204.000	37090.000	326.940556	179654.389	191768.389	472090.000	-243231.611
800.00	124.12000	61231.000	49117.000	342.990556	213161.445	225275.445	484117.000	-209724.555
900.00	130.81000	73990.000	61876.000	358.010556	248219.500	260333.500	496876.000	-174666.500
1000.00	136.50000	87360.000	75246.000	372.090556	284730.556	296844.556	510246.000	-138155.444
1100.00	141.50000	101260.000	89146.000	385.390556	322669.612	334783.612	524146.000	-100216.338
1200.00	145.70000	115630.000	103516.000	397.890556	361838.667	373952.667	538516.000	-61047.333
1300.00	149.40000	130390.000	118276.000	409.690556	402207.723	414321.723	553276.000	-20678.277
1400.00	152.70000	145500.000	133386.000	420.890556	443746.779	455860.779	568386.000	20860.779
1500.00	155.50000	160920.000	148806.000	431.490556	486315.834	498429.834	583806.000	63429.834
1600.00	157.10409	176521.795	164407.795	441.558953	529972.529	542086.529	599407.795	107086.529
1800.00	160.76845	208324.442	196210.442	460.283781	620186.363	632300.363	631210.442	197300.363
2000.00	163.64548	240776.921	228662.921	477.377171	713977.420	726091.420	663662.921	291091.420
2200.00	165.94873	273744.528	261630.528	493.086170	811045.047	823159.047	696650.528	388159.047
2400.00	167.82394	307127.971	295013.971	507.608685	911132.872	923246.872	730013.971	488246.872
2600.00	169.37318	340852.435	328738.435	521.104845	1014020.162	1026134.162	763738.435	591134.162
2800.00	170.66967	374860.437	362746.437	533.705572	1119515.165	1131629.165	797746.437	696629.165
3000.00	171.76700	409107.056	396993.056	545.519000	1227449.944	1239563.944	831993.056	804563.944
3200.00	172.70516	443556.648	431442.648	556.635303	1337676.322	1349790.322	866442.648	914790.322
3400.00	173.51449	478180.548	466066.548	567.130359	1450062.674	1462176.674	901066.548	1027176.674
3600.00	174.21832	512955.422	500841.422	577.068551	1564491.362	1576605.362	935841.422	1141605.362
3800.00	174.83490	547862.069	535748.069	586.504928	1680856.657	1692970.657	970748.069	1257970.657
4000.00	175.37861	582884.530	570770.530	595.486896	1799063.053	1811177.053	1005770.530	1376177.053
4200.00	175.86095	618009.425	605895.425	604.055547	1919023.872	1931137.872	1040895.425	1496613.872
4400.00	176.29122	653225.443	641111.443	612.246718	2040660.116	2052774.116	1076111.443	1617774.116
4600.00	176.67697	688522.949	676408.949	620.091836	2163899.498	2176013.498	1111408.949	1741013.498
4800.00	177.02442	723893.680	711779.680	627.618607	2288675.634	2300789.634	1146779.680	1865789.634
5000.00	177.33871	759330.507	747216.507	634.851573	2414927.359	2427041.359	1182216.507	1992041.359

ORIGINAL ATM CYCLOBUTADIENE

Example 4 (C₅H₁₁(g) by Method RRHO with Internal Rotation)

Problem.—Calculate thermodynamic properties for a species with internal rotation using the RRHO method.

The comments for this species will be mainly with respect to the method (METH RRHO) and the data records. The remaining records are similar to those discussed in the first three examples. The method RRHO is the rigid rotator-harmonic oscillator approximation. Please refer to tables II and VII for the required data. The tert-pentyl radical is a nonlinear molecule and thus has a total of $3N-6$ fundamental frequencies ($V_i(d_i)$ values) and internal rotors (INTROT value), where N is the number of atoms in the molecule. In this case the number is $3(16)-6 = 42$, with 38 frequencies and four rotors. Fourteen unique frequencies are given on the data records with their multiplicities given in parentheses. The rigid rotator part requires either the moments of inertia (IA,IB,IC)

or rotational constants (A0,B0,C0) for the nonlinear molecule. For this example the individual moments of inertia in $(g)(cm)^2 \times 10^{39}$ have been multiplied together into one value of 8590. with the label IAIBIC.

The four internal rotors are specified by the label INTROT and its corresponding numerical value of 4.. (Note that the record ID on the data records are all blank, which is one of the permitted options.) The data records for the individual rotors are identified by the number in column 80. The third and fourth rotors for C₅H₁₁ have identical parameters so they may be combined by using NROTOR = 2. on the data record for the third rotor. The barrier potential for the first rotor is $V_3 = 1254. \text{ cm}^{-1}$. Inasmuch as no potentials are specified for the other rotors, the program treats them as free rotors. The IB values for the rotors are the moments of inertia in $(g)(cm)^2 \times 10^{39}$ and the ROSYM values are the symmetry numbers for the rotors.

Input. - The input data set for C₅H₁₁, example 4, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79 - 80
a	NAME	TERT-PENTYL RAD	WING TSANG, J.A.M.C.H.SOC.,	MAY 15,1985, P2872.	Exp1.	4			
	C5H11		HF298	32600.	JOULES				
a	DATE	L 5/87							
a	REFN	WING TSANG, 'THE STABILITY OF ALKYL	RADICALS,' J. AM. CHEM. SOC.						
	REFN	MAY 15,1985, PP 2872-2880.							
	TEMP	T 100.	T 1000.	I	1000.	T	6000.		
	OUTP	MFIG	DMLESS	JOULES		CAL			
	METH	RRHO							
		V1(9)	V2(2)	2825.	V3(8)	1455.	V4(3)	1370.	
		V5	V6(2)	1252.	V7(2)	1189.	V8	1126.	
		V9(3)	V10	733.	V11(2)	541.	V12	380.	
		V13(1)	V14(2)	990.	STATWT	2.	IAIBIC	8590.	
		INTROT 4.							
		NEL 100.			NROTOR	1.			1
		ROSYM 3.	V3	1254.	IB	.48			1
		ROSYM 1.	NROTOR	1.	IB	2.1			2
		ROSYM 3.	NROTOR	2.	IB	.48			3
	FINISH								

^aAll alphanumeric characters.

Listed output. - Listed output for C₅H₁₁, example 4, is as follows:

```

NAME TERT-PENTYL RAD WING TSANG, J.AM.CHEM.SOC., MAY 15,1985, P2872. Exp1. 4
C5H11 HF298 32600. JOULES
DATE L 5/87
REFN WING TSANG, 'THE STABILITY OF ALKYL RADICALS,' J. AM. CHEM. SOC.
REFN MAY 15,1985, PP 2872-2880.
TEMP T 100. T 1000. I 1000. T 6000.
DUIP MFIG DMLESS JOULES CAL
METH RRHO
MOLECULAR WT.= 71.14234
V1(9) 2931. V2(2) 2825. V3(8) 1455. V4(3) 1370.
V5 1279. V6(2) 1252. V7(2) 1189. V8 1126.
V9(3) 992. V10 733. V11(2) 541. V12 380.
V13(1) 200. V14(2) 990. STATHT 2. IAIBIC 8590.
INTROT 4.
NEL 100. NROTOR 1. 1
ROSYM 3. V3 1254. IB .48 1
ROSYM 1. NROTOR 1. IB 2.1 2
MINIMUM OF POTENTIAL FUNCTION IS 0.000 CM**(-1)
BARRIER POTENTIAL CONSTANTS IN CAL/MOL 0.00 0.00 3585.37 0.00 0.00 0.00
OR IN CM**(-1) 0.000 0.000 1254.000 0.000 0.000 0.000
ROTATION CONSTANTS IN CM**(-1) 5.83183 0.00000 0.00000 0.00000
ROSYM 3. NROTOR 2. IB .48 3
V=0 FOR ROTOR 2. USE CLASSICAL PARTITION FUNCTION FOR FREE ROTOR (IROTOR).
F.I.G.H
V=0 FOR ROTOR 3. USE CLASSICAL PARTITION FUNCTION FOR FREE ROTOR (IROTOR).
ORIGINAL BAR TERT-PENTYL RAD

ORIGINAL TERT-PENTYL RAD
ASSIGNED H/R AT 0 K = 1558.273 K
T CP/R (H-H0)/RT (H-H298)/RT S/R -(G-H0)/RT -(G-H298)/RT H/RT -G/RT
100.00 6.60920 5.8128262 -17.8130086 34.7528978 28.9400716 52.5659063 21.3955557 13.3573420
298.15 11.88955 7.9241438 0.0000000 44.0766593 36.1525155 44.0766593 33.1506169 30.9260424
1000.00 30.82205 18.3487024 15.9861190 69.2977936 50.9490911 53.3116746 19.9069754 49.3908182
2000.00 39.26581 27.1681671 25.9868754 93.9084148 66.7402477 67.9215594 27.9473036 65.9611112
3000.00 41.70940 31.6782837 30.8907559 110.3772014 78.6989178 79.4864456 32.1977080 78.1794934
4000.00 42.67036 34.3221130 33.7514672 122.5262009 88.2040879 88.7947338 34.7116813 87.8145177
5000.00 43.13628 36.0433197 35.5708030 132.1034232 96.0601035 96.5326202 36.3549743 95.7484439
6000.00 43.39522 37.2489471 36.8551832 139.9930650 102.7441179 103.1378818 37.5086593 102.4844057

ORIGINAL TERT-PENTYL RAD
ASSIGNED H AT 0 K = 12956.276 J/MOLE
T DEG-K CP J/MOL-K H-H0 J/MOL H-H298 J/MOL S J/MOL-K -(G-H0) J/MOL -(G-H298) J/MOL H J/MOL -G J/MOL
100.00 54.95223 4833.080 -14810.644 288.953316 24062.251 43705.975 17789.356 11105.975
298.15 98.85578 19843.724 0.000 366.475825 89621.043 109264.767 32600.000 76664.767
1000.00 256.27026 152560.470 132916.746 576.177198 423616.728 443260.452 165516.746 410660.452
2000.00 326.47595 451779.994 432136.270 780.802454 1109824.913 1129468.637 464736.270 1096868.637
3000.00 346.79319 790168.220 770524.496 917.732345 1963028.816 1982672.540 803124.496 1950072.540
4000.00 354.78317 1141486.208 1121842.484 1018.745323 2933495.084 2953138.807 1154442.484 2920538.807
5000.00 358.65700 1498412.710 1478768.987 1098.375233 3993463.456 4015107.180 1511368.987 3980507.180
6000.00 360.80997 1858240.461 1838596.737 1163.973739 5125601.972 5145245.696 1871196.737 5112645.696

ORIGINAL TERT-PENTYL RAD
ASSIGNED H AT 0 K = 3096.624 CAL/MOLE
T DEG-K CP CAL/MOL-K H-H0 CAL/MOL H-H298 CAL/MOL S CAL/MOL-K -(G-H0) CAL/MOL -(G-H298) CAL/MOL H CAL/MOL -G CAL/MOL
100.00 13.13390 1155.154 -3539.829 69.061500 5751.016 10445.979 4251.758 2654.392
298.15 23.62710 3694.963 0.000 87.589824 21419.943 26114.906 7791.587 18323.319
1000.00 61.25006 36462.827 31767.865 137.709655 101246.828 105941.791 39559.452 98150.204
2000.00 78.02963 107978.010 103283.047 186.616265 265254.520 269949.483 111074.634 262157.896
3000.00 82.88556 188856.757 184159.774 219.343295 469175.147 473870.110 191951.361 466078.523
4000.00 84.79521 272821.751 268126.789 243.485976 701122.152 705817.115 275918.376 698025.528
5000.00 85.72108 350129.233 353434.270 262.517981 954460.673 959155.636 361225.857 951364.049
6000.00 86.23565 444130.129 439435.167 278.196400 1225048.273 1229743.235 447226.754 1221951.648

ORIGINAL BAR TERT-PENTYL RAD

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Example 5 (H₂O(g) by Method NRRAO2 with Intermediate Output)

Problem.—Calculate thermodynamic functions for H₂O(g) using method NRRAO2. List some intermediate results in addition to final tables.

This is the only one of the eight examples discussed which does not start with a NAME record. This optional record was intentionally omitted to show that, as a result, the output tables are not identified by species name on the bottom of the listings. Therefore, while the NAME record is optional, it is generally useful to include it.

A REFNCE record was used to indicate the example number. This is followed by the formula record. It gives the formula with all the stoichiometric coefficients and an assigned enthalpy (ASINDH) of -57103.5 cal/mol (CAL) at $T = 0$ K. The TEMP record indicates a temperature schedule of only one value, 5000 K. The OUTP record calls for intermediate output (INTERM) and a many-figured table (MFIG) in energy units of joules (JOULES).

The NRRAO1 and NRRAO2 methods are the only methods in PAC91 that can accommodate the large variety of spectroscopic constants available for H₂O(g). In addition to the fundamental frequencies ν_i and rotational constants A_0 , B_0 , and C_0 , other constants included are the anharmonicities x_{ij} and y_{ijk} ; vibration-rotation interaction constants α_i^A (ALFAAi), α_i^B (ALFABi), and α_i^C (ALFACi) for $i = 1, 2$ and 3 ; rotation-stretching constant ρ ; and symmetry number (SYMNO). These spectroscopic constants appear on the nine data records following the METHOD NRRAO2 record. The FINISH record is last, as usual.

The intermediate output follows the input record images for each electronic state plus one record. For this case there is only the ground state and the intermediate output follows the FINISH record. This output is discussed in section **Intermediate data with INTERM label** in appendix C. The last item listed is the many-figured table with properties at 5000 K and energy units in joules.

Input. - The input data set for H₂O, example 5, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79- 80
a	REFNCE							Expl.	5
	H2O1		ASINDH	-57103.5	CAL		T	0.	
	TEMP	5000.							
	OUTP	INTERM	MFIG		JOULES				
	METHOD		NRRAO2						
	DATA	V1	V2	1594.78	V3	3755.79	X11	-45.18	
	DATA	X12	X33	-44.62	X13	-165.48	X22	-17.04	
	DATA	Y233	Y333	-.45	X23	-19.99			
	DATA	Y111	Y112	-.10	Y113	.68	Y122	-0.1	
	DATA	Y123	Y133	1.17	Y222	-.60	Y223	1.55	
	DATA	A0	B0	14.5064	C0	9.28285	SYMNO	2.	
	DATA	ALFAA1	ALFAA2	-2.941	ALFAA3	1.253	ALFAB1	.238	
	DATA	ALFAB2	ALFAB3	.078	ALFAC1	.2018	ALFAC2	.1392	
	DATA	ALFAC3	RHO	.0000213	STATWT	1.			
	FINISH								

^aAll alphanumeric characters.

Listed output. - The listed output for H₂O, example 5, is as follows:

```

REFNCE                               Expl. 5
H2O1                                ASINDH -57103.5  CAL      T      0.
TEMP T      5000.
OUTP INTERM      MFIG                JOULES
METHOD      NRRA02
MOLECULAR WT.= 18.01528
DATA V1 3656.65 V2 1594.78 V3 3755.79 X11 -45.18
DATA X12 -15.14 X33 -44.62 X13 -165.48 X22 -17.04
DATA Y233 -.81 Y333 -.45 X23 -19.99
DATA Y111 .47 Y112 -.10 Y113 .68 Y122 -0.1
DATA Y123 -1.72 Y133 1.17 Y222 -.60 Y223 1.55
DATA A0 27.848 B0 14.5064 C0 9.28285 SYMNO 2.
DATA ALFAA1 .750 ALFAA2 -2.941 ALFAA3 1.253 ALFAB1 .238
DATA ALFAB2 -.160 ALFAB3 .078 ALFAC1 .2018 ALFAC2 .1392
DATA ALFAC3 .1445 RHO .0000213 STATWT 1.
FINISH
AI = 0.0325387 ALPHA A = 0.7500000 ALPHA B = 0.2380000 ALPHA C = 0.2018000 I = 1
AI = -0.0508216 ALPHA A = -2.9410000 ALPHA B = -0.1600000 ALPHA C = 0.1392000 I = 2
AI = 0.0329687 ALPHA A = 1.2529993 ALPHA B = 0.0779999 ALPHA C = 0.1445000 I = 3
THETA(1) = 4.448227 THETA(2) = 19.370178 THETA(3) = 0.000000
A0= 27.847992 B0= 14.506399 C0= 9.282849
IAIBIC= 0.005849E-117 (G*CM**2)**3
Y(1,1,1) = 0.470 Y(1,1,2) = -0.100 Y(1,1,3) = 0.680 Y(1,2,2) = -0.100 Y(1,2,3) = -1.720
Y(1,3,3) = 1.170 Y(2,2,2) = -0.600 Y(2,2,3) = 1.550 Y(2,3,3) = -0.810 Y(3,3,3) = -0.450
X(I,J)
-42.7750 -16.4000 -162.6400
-16.4000 -19.0150 -19.3700
-162.6400 -19.3700 -46.4650
V( 1) =3656.6499(1) G = 0.000
V( 2) =1594.7798(1) G = 0.000
V( 3) =3755.7898(1) G = 0.000
T = 5000.000
U = 0.1052215e+01 R = 0.3491637e+00 S = 0.1536484e+01 I = 1
U = 0.4589038e+00 R = 0.6319761e+00 S = 0.2717215e+01 I = 2
U = 0.1080742e+01 R = 0.3393437e+00 S = 0.1513646e+01 I = 3
CONTRIBUTION      Q      LN Q      H-H0/RT      CP/R
ELEC      0.5000e+00      -0.69314718      0.00000000      0.00000000
H.O.      0.6319e+01      1.84362507      1.90765095      2.80335808
R.R.      0.5930e+04      8.68771458      1.50000000      1.50000000
RHO      0.1112e+01      0.10649991      0.10649991      0.21299982
THTA      0.1001e+01      0.00088938      -0.00089040      0.00000076
FIRST ORDER CORRECTIONS
ALFA      0.9546e+00      -0.04642935      -0.04005833      -0.06193634
XIJJ      0.1071e+01      0.06857038      0.12646741      0.30334258
YIJK      0.1004e+01      0.00428620      0.01142810      0.03873271
AXIJ      0.9930e+00      -0.00702811      -0.01502087      -0.04562024
SECOND ORDER CORRECTIONS
XIJJ2      0.1010e+01      0.00975084      0.02659326      0.09222138
XY      0.1003e+01      0.00264854      0.00939406      0.04116780
AX2      0.9977e+00      -0.00226233      -0.00755092      -0.03202931
ORIGINAL
ASSIGNED H AT 0 K = -238921.044 J/MOLE
T      CP      H-H0      H-H298      S      -(G-H0)      -(G-H298)      H      -G
DEG-K  J/MOL-K  J/MOL  J/MOL  J/MOL-K  J/MOL  J/MOL  J/MOL  J/MOL
5000.00  61.13024  254611.490  316.597784  1328377.430  15690.446  1567298.474

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ORIGINAL BAR

Example 6 (Mg(cr,l) by Methods READIN and COEF with EFTAPE and LSQS Options)

Problem.—Process data for an assigned reference element to illustrate preparation of EF data. Select an element with more than one condensed phase in temperature range of interest. The solid phase is in the crystalline form and this is indicated on the NAME record as Mg(cr). Also obtain least-squares coefficients for each phase.

Magnesium in the solid and liquid phases was chosen to be the assigned reference element. Referring to the input data set, there is a NAME record for each phase. The information on these records will be included with the first record of the least-squares coefficients output on I/O units 6 and 10. See the section **NAME record** in appendix B and table VIII. The formula record contains the atomic symbol in the required capital letters, the integer 1 and the letter S in parentheses. The parentheses are a requirement for condensed species. As was noted in the section **Formula record**, the letter S must be used on the formula record of a reference element to specify the solid state. However, a more descriptive letter (or letters) such as cr may be used in the NAME record. Also included on the formula record is the assigned enthalpy at 298.15 K (HF298) which is 0 since this is a reference element. The CODA89 label on the DATE record was chosen to indicate a 1989 CODATA reference. The four REFN records give the full reference and some comments on the data.

The two OUTF records list many options. The EFTAPE label calls for the enthalpy and Gibbs energy data (EF data) to be merged in an unformatted form with the data on I/O unit 13 for use in calculating $\Delta_f H_T^\circ$ and $\log_{10} K$ values for future calculations. The data are also listed in formatted form on I/O units 11 and 6 (see the second to last table for this example printed in the output below). More discussion is given in the section **Saved Output** in appendix C. The LSQS label calls for least-squares coefficients. The MFIG label calls for many-figured tables with joules as the energy unit (JOULES). The CTAB label calls for a table to be listed for data calculated from the least-squares coefficients. The temperature schedule for the *coefficients* table is given on the CTEM record—namely, from 200 to 5000 K in 200 K intervals. Room temperature (298.15 K) and phase transition temperatures are always inserted by the PAC91 program in these schedules.

Data for the solid phase (Mg(s)) are processed by method READIN, whereas data for the liquid phase are processed by method COEF. The 18 data records (indicated by record ID MG- SOL) give data for the solid phase from 25 to 923 K. The melting point is given on the METHOD record as 923.. Also given on this record is the H298H0 value of 4998.. The

unit of J/mol is specified by the label JOULES. Note that some of the enthalpy values are for H-H0 ($H_T^\circ - H_0^\circ$) whereas others are for H-H2 ($H_T^\circ - H_{298.15}^\circ$). This was done just to demonstrate some of the options available.

The heat of melting is given on the second METHOD record (method COEF for the liquid phase) as DELTAH = 8477. J/mol. The temperature schedule for thermodynamic functions calculated from read-in coefficients is given on the TEMP record preceding the COEF method record. Following this METHOD record are two data records for the liquid phase (records MG-LIQ). The first MG-LIQ record contains one coefficient (C1 = 34.309), one exponent (E1 = 0.), and the temperature range for which these coefficients are valid (923 to 6000 K). The PAC91 program automatically prepares and lists the read-in coefficients in the same format as the least-squares coefficients (see table VIII). The TCOEF label (on the second MG-LIQ data record for the liquid phase) has no temperature information following it. Therefore, the temperature range for the liquid phase on the coefficient output just discussed is taken to be the same as the input temperature range for the liquid.

As the listed output below shows, the least-squares calculations for the crystalline phase were done by PAC91 after reading the METHOD COEF record and before processing the liquid data records. This is evidenced by the intermediate output for the least-squares fit for the crystalline phase. Since no LSTSQS records were included in the input, the default parameters are used. The temperature interval starts at 200 K and ends at the 923 K transition which comes ahead of the 1000 K midpoint. The functions are fit simultaneously and constrained to fit at 298.15 K. The equation is the default seven-coefficient function for C_p° (see eq. (17)). The record images described in table VIII are printed here (I/O unit 6) and on I/O unit 10.

This output is followed by the input data images for the liquid (record ID MG-LIQ). The TCOEF label indicates that the coefficients on the data records are to be included with the least-squares coefficients. In this case there is one coefficient for the constant C_p° . The two required integration constants for enthalpy and entropy are calculated by PAC91 to fit the properties calculated from the least-squares coefficients for the solid phase at 923 K plus the heat of melting. These coefficients are also written on I/O unit 6 following the FINISH record as well as on I/O unit 10. No least-squares calculations were made for the liquid since the TCOEF option was used.

The final three tables are in order: the many-figured *original* table in SI units, the dimensionless EF data, and the many-figured *coefficient table* in SI units.

Input. - The input data set for Mg(cr,l), example 6, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79 - 80
a	NAME	Mg(cr)		Magnesium Hexagonal	Crystal.	CODATA	1989,	p244.	Expl. 6
a	NAME	Mg(l)		Magnesium Liquid.		CODATA	1989, p244.		
	MG1(S)		HF298	0.					
	DATE	CODA89							
a	REFN	Cox, J.D.; Wagman, D.D.; and Medvedev, V.A.:				CODATA Key Values for			
a	REFN	Thermodynamics.				Hemisphere Publ. Corp., 1989.			
a	REFN	CODATA S value at 75 K was obviously wrong and corrected by interpolation.							
a	REFN	H and S for crystal at 923 adjusted so rounded liq values match CODATA.							
	OUTP	EFTAPE	MFIG		JOULES		LSQS		
	OUTP	CTAB							
	CTEM	T							
	METHOD	READIN	I	200.	T	6000.			
	MG-SOLT	25.	H298H0	4998.	JOULES		MELTPT	923.	
	MG-SOLT	50.	CP	0.781	S	.246	H-H0	5.	
	MG-SOLT	75.	CP	5.740	S	2.104	H-H0	79.	
	MG-SOLT	100.	CP	11.542	S	5.578	H-H0	297.	
	MG-SOLT	150.	CP	15.762	S	9.505	H-H2	-4356.	
	MG-SOLT	200.	CP	20.474	S	16.910	H-H0	1563.	
	MG-SOLT	250.	CP	22.724	S	23.143	H-H2	-2349.	
	MG-SOLT	298.15	CP	24.018	S	28.364	H-H0	3820.	
	MG-SOLT	300.	CP	24.869	S	32.671	H-H2	0000.	
	MG-SOLT	350.	CP	24.897	S	32.825	H-H2	46.	
	MG-SOLT	400.	CP	25.568	S	36.715	H-H0	6306.	
	MG-SOLT	450.	CP	26.144	S	40.167	H-H2	2601.	
	MG-SOLT	500.	CP	26.668	S	43.277	H-H0	8920.	
	MG-SOLT	600.	CP	27.171	S	46.113	H-H2	5268.	
	MG-SOLT	700.	CP	28.184	S	51.156	H-H2	8035.	
	MG-SOLT	800.	CP	29.279	S	55.581	H-H2	10907.	
	MG-SOLT	900.	CP	30.507	S	59.569	H-H2	13895.	
	MG-SOLT	923.	CP	31.895	S	63.241	H-H2	17014.	
	TEMP	T		32.238	S	64.0498	H-H2	17751.2	
	METHOD	COEF	T	1000.	I	100.	T	6000.	
	MG-LIQT	923.	DELTAH	8477.	JOULES				
	MG-LIQT	COEF	T	6000.	C1	34.309	E1	0.	
	FINISH								

^aAll alphanumeric characters.

Listed output. - Listed output for Mg(cr,0), example 6, is as follows:

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NAME Mg(cr)           Magnesium Hexagonal Crystal. CODATA 1989, p244.  Expl. 6
NAME Mg(l)           Magnesium Liquid. CODATA 1989, p244.
MGL(S)              HF298      0.
DATE CODA89
REFN Cox,J.D.; Hagman, D.D.; and Medvedev,V.A.: CODATA Key Values for
REFN Thermodynamics. Hemisphere Publ. Corp., 1989.
REFN CODATA S value at 75 K was obviously wrong and corrected by interpolation.
REFN H and S for crystal at 923 adjusted so rounded liq values match CODATA.
OUTP EFTAPE          MFIG              JOULES              LSQS
OUTP CTAB
CTEM T              200.              I              200.              T              6000.
METHODREADIN        H298H0 4998.          JOULES              MELTPT 923.
MG-SOLT              25.              CP              0.781              S              .246              H-H0              5.
MG-SOLT              50.              CP              5.740              S              2.104              H-H0              79.
MG-SOLT              75.              CP              11.542             S              5.578              H-H0              297.
MG-SOLT              100.             CP              15.762              S              9.505              H-H2             -4356.
MG-SOLT              150.             CP              20.474              S              16.910             H-H0             1563.
MG-SOLT              200.             CP              22.724              S              23.143             H-H2             -2349.
MG-SOLT              250.             CP              24.018              S              28.364             H-H0             3820.
MG-SOLT              298.15           CP              24.869              S              32.671             H-H2             0000.
MG-SOLT              300.             CP              24.897              S              32.825             H-H2              46.
MG-SOLT              350.             CP              25.568              S              36.715             H-H0             6306.
MG-SOLT              400.             CP              26.144              S              40.167             H-H2             2601.
MG-SOLT              450.             CP              26.668              S              43.277             H-H0             8920.
MG-SOLT              500.             CP              27.171              S              46.113             H-H2             5268.
MG-SOLT              600.             CP              28.184              S              51.156             H-H2             8035.
MG-SOLT              700.             CP              29.279              S              55.581             H-H2            10907.
MG-SOLT              800.             CP              30.507              S              59.569             H-H2            13895.
MG-SOLT              900.             CP              31.895              S              63.241             H-H2            17014.
MG-SOLT              923.             CP              32.238              S              64.0498            H-H2            17751.2
TEMP T              923.              T              1000.              I              100.              T              6000.
METHODCOEF          DELTAH 8477.          JOULES

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LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
200.00	2.7330534	2.7329970	1.5929983	1.5928976	2.7834473	2.7834025	1.1904490	1.1905050
250.00	0.0000564	0.0000206	0.0001007	0.0000632	0.0000447	0.0000161	-0.0000560	-0.0000470
298.15	2.8886850	2.8889734	1.8377511	1.8377226	3.4113856	3.4113582	1.5736345	1.5736357
300.00	-0.0002884	-0.0000998	0.0000286	0.0000155	0.0000274	0.0000080	-0.0000011	-0.0000007
350.00	2.9944038	2.9944025	2.0221677	2.0221811	3.9293957	3.9293957	1.9152367	1.9152367
400.00	0.0000012	0.0000004	-0.0000135	-0.0000067	0.0000000	0.0000000	0.0000000	0.0000000
450.00	3.0751060	3.0755575	2.1669519	2.1670665	4.4157746	4.4158074	1.9257499	1.9257263
500.00	-0.0004514	-0.0001468	-0.0001146	-0.0000529	-0.0000330	-0.0000075	0.0000231	0.0000120
550.00	3.1443825	3.1444155	2.2848610	2.2850201	4.8309522	4.8310806	2.2488225	2.2487409
600.00	-0.0000330	-0.0000105	-0.0001590	-0.0000696	-0.0001285	-0.0000266	0.0000816	0.0000365
650.00	3.2074049	3.2072398	2.3840518	2.3840347	5.2049970	5.2051049	2.5460911	2.5460605
700.00	0.0001651	0.0000515	0.0000170	0.0000071	-0.0001078	-0.0000207	0.0000306	0.0000129
750.00	3.2679015	3.2676623	2.4694179	2.4693854	5.5460875	5.5461580	2.8209453	2.8210701
800.00	0.0002393	0.0000732	0.0000325	0.0000132	-0.0000705	-0.0000127	-0.0001249	-0.0000443
850.00	3.3897367	3.3896968	2.6125011	2.6125225	6.1526175	6.1526248	3.0766696	3.0767727
900.00	0.0000399	0.0000118	-0.0000213	-0.0000082	-0.0000073	-0.0000012	-0.0001031	-0.0000335
923.00	3.5214342	3.5215153	2.7327442	2.7328045	6.6848197	6.6848772	3.5401164	3.5401023
	-0.0000811	-0.0000230	-0.0000604	-0.0000221	-0.0000576	-0.0000086	0.0000028	0.0000007
	3.6691278	3.6690433	2.8403658	2.8404281	7.1644631	7.1645425	4.3240973	4.3241144
	0.0000845	0.0000230	-0.0000623	-0.0000219	-0.0000794	-0.0000111	-0.0000171	-0.0000040
	3.8360649	3.8359739	2.9415778	2.9415776	7.6061007	7.6061272	4.6645229	4.6645495
	0.0000910	0.0000237	0.0000002	0.0000001	-0.0000265	-0.0000035	-0.0000267	-0.0000057
	3.8773181	3.8773931	2.9643583	2.9643784	7.7033764	7.7034439	4.7390381	4.7390654
	-0.0000750	-0.0000193	-0.0000401	-0.0000135	-0.0000675	-0.0000088	-0.0000274	-0.0000053
MAX REL ERR CP/R = 0.000147 TEMP = 350. AVER REL ERR CP/R = 0.000039 REL LST SQ ERR CP/R = 0.000057 MAX REL ERR HH/RT = 0.000070 TEMP = 400. AVER REL ERR HH/RT = 0.000023 REL LST SQ ERR HH/RT = 0.000032 MAX REL ERR S/R = 0.000027 TEMP = 400. AVER REL ERR S/R = 0.000010 REL LST SQ ERR S/R = 0.000012 MAX REL ERR GH/RT = 0.000047 TEMP = 200. AVER REL ERR GH/RT = 0.000016 REL LST SQ ERR GH/RT = 0.000023 MAX REL CP/R = 0.000451 TEMP = 350. AVER REL CP/R = 0.000124 LST SQ ERR CP/R = 0.000177 MAX REL HH/RT = 0.000159 TEMP = 400. AVER REL HH/RT = 0.000050 LST SQ ERR HH/RT = 0.000068 MAX REL S/R = 0.000128 TEMP = 400. AVER REL S/R = 0.000051 LST SQ ERR S/R = 0.000063 MAX REL GH/RT = 0.000125 TEMP = 450. AVER REL GH/RT = 0.000039 LST SQ ERR GH/RT = 0.000055 CP/R = -7.3557794e+031**2.0 -6.9826242e+011**1.0 3.2083651e+001**0.0 2.2508743e-041**1.0 2.0515951e-071**2.0 5.6911578e-101**3.0 -1.0573239e-131**4.0 (H-H0)/R CONSTANT = 0.48294728e+01, H/R CONSTANT =-0.59628833e+03, S/R CONSTANT =-0.14707183e+02								

Mg(cr) Mg(l)

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

Mg(cr) Magnesium Hexagonal Crystal. CODATA 1989, p244. Expl. 6
 1 CODA89 MG 1.00 0.00 0.00 0.00 0.00 1 24.30500 0.000
 200.000 923.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4998.000
 -7.35377939d+03 -6.98262416d+01 3.20836507d+00 2.25087426d-04 2.05159514d-07
 5.69115784d-10 -1.05732390d-13 0.00000000d+00 -5.96288332d+02 -1.47071833d+01

MG-LIQT 923. T 6000. C1 34.309 E1 0.

MG-LIQTCOEF

FINISH

COEFFICIENTS ADJUSTED TO FIT UPPER PHASE AT 923.00

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

Mg(l) Magnesium Liquid. CODATA 1989, p244.
 1 CODA89 MG 1.00 0.00 0.00 0.00 0.00 2 24.30500 0.000
 923.000 6000.000 1 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 4998.000
 4.12640071d+00 0.00000000d+00 0.00000000d+00 0.00000000d+00 0.00000000d+00
 0.00000000d+00 0.00000000d+00 0.00000000d+00 -6.54121412d+02 -1.93654933d+01

ORIGINAL Mg(cr) Mg(l)
 ASSIGNED H AT 0 K = -4998.000 J/MOLE

T DEG-K	CP J/MOL-K	H-HO J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-HO) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
25.00	0.78100	5.000	-4993.000	0.246000	1.150	4999.150	-4993.000	4999.150
50.00	5.74000	79.000	-4919.000	2.104000	26.200	5024.200	-4919.000	5024.200
75.00	11.54200	297.000	-4701.000	5.578000	121.350	5119.350	-4701.000	5119.350
100.00	15.76200	642.000	-4356.000	9.505000	308.500	5306.500	-4356.000	5306.500
150.00	20.47400	1563.000	-3435.000	16.910000	973.500	5971.500	-3435.000	5971.500
200.00	22.72400	2649.000	-2349.000	23.143000	1979.600	6977.600	-2349.000	6977.600
250.00	24.01800	3820.000	-1178.000	28.364000	3271.000	8269.000	-1178.000	8269.000
298.15	24.86900	4984.000	0.000	32.671000	4742.859	9740.859	0.000	9740.859
300.00	24.89700	5044.000	46.000	32.825000	4803.500	9801.500	46.000	9801.500
350.00	25.56800	6306.000	1308.000	36.715000	6544.250	11542.250	1308.000	11542.250
400.00	26.14400	7599.000	2601.000	40.167000	8467.800	13465.800	2601.000	13465.800
450.00	26.66800	8920.000	3922.000	43.277000	10554.650	15552.650	3922.000	15552.650
500.00	27.17100	10266.000	5268.000	46.113000	12790.500	17788.500	5268.000	17788.500
600.00	28.18400	13033.000	8035.000	51.156000	17660.600	22658.600	8035.000	22658.600
700.00	29.27900	15905.000	10907.000	55.581000	23001.700	27999.700	10907.000	27999.700
800.00	30.50700	18893.000	13895.000	59.569000	28622.200	33760.200	13895.000	33760.200
900.00	31.89500	22012.000	17014.000	63.241000	34904.900	39902.900	17014.000	39902.900
923.00	32.23800	22749.200	17751.200	64.049800	36368.765	41366.765	17751.200	41366.765
923.00	34.30900	31226.200	26228.200	73.233982	36368.765	41366.765	26228.200	41366.765
1000.00	34.30900	33867.993	28869.993	75.983026	42115.033	47113.033	28869.993	47113.033
1100.00	34.30900	37298.893	32300.893	79.253023	49879.433	54877.433	32300.893	54877.433
1200.00	34.30900	40729.793	35731.793	82.238297	57956.163	62954.163	35731.793	62954.163
1300.00	34.30900	44160.693	39162.693	84.984482	66319.134	71317.134	39162.693	71317.134
1400.00	34.30900	47591.593	42593.593	87.527052	74946.280	79944.280	42593.593	79944.280
1500.00	34.30900	51022.493	46024.493	89.894129	83818.700	88816.700	46024.493	88816.700
1600.00	34.30900	54453.393	49455.393	92.108381	92920.017	97918.017	49455.393	97918.017
1700.00	34.30900	57884.293	52886.293	94.188351	102235.904	107235.904	52886.293	107235.904
1800.00	34.30900	61315.193	56317.193	96.149399	111753.725	116751.725	56317.193	116751.725
1900.00	34.30900	64746.093	59748.093	98.004391	121462.251	126460.251	59748.093	126460.251
2000.00	34.30900	68176.993	63178.993	99.764213	131351.433	136349.433	63178.993	136349.433
2100.00	34.30900	71607.893	66609.893	101.438155	141412.232	146410.232	66609.893	146410.232
2200.00	34.30900	75038.793	70040.793	103.034210	151636.469	156634.469	70040.793	156634.469
2300.00	34.30900	78469.693	73471.693	104.559306	162016.710	167014.710	73471.693	167014.710
2400.00	34.30900	81900.593	76902.593	106.019483	172546.167	177544.167	76902.593	177544.167
2500.00	34.30900	85331.493	80333.493	107.420045	183218.620	188216.620	80333.493	188216.620
2600.00	34.30900	88762.393	83764.393	108.765669	194028.345	199026.345	83764.393	199026.345
2700.00	34.30900	92193.293	87195.293	110.060502	204970.061	209968.061	87195.293	209968.061
2800.00	34.30900	95624.193	90626.193	111.308578	216038.876	221036.876	90626.193	221036.876
2900.00	34.30900	99055.093	94057.093	112.512187	227230.250	232228.250	94057.093	232228.250
3000.00	34.30900	102485.993	97487.993	113.675315	238559.953	243557.953	97487.993	243557.953
3100.00	34.30900	105916.893	100918.893	114.800302	249964.042	254962.042	100918.893	254962.042
3200.00	34.30900	109347.793	104349.793	115.889568	261498.823	266496.823	104349.793	266496.823
3300.00	34.30900	112778.693	107780.693	116.945312	273140.838	278138.838	107780.693	278138.838
3400.00	34.30900	116209.593	111211.593	117.969538	284886.835	289884.835	111211.593	289884.835
3500.00	34.30900	119640.493	114642.493	118.964071	296733.756	301731.756	114642.493	301731.756
3600.00	34.30900	123071.393	118073.393	119.930586	308678.716	313676.716	118073.393	313676.716
3700.00	34.30900	126502.293	121504.293	120.870617	320718.991	325716.991	121504.293	325716.991
3800.00	34.30900	129933.193	124935.193	121.785578	332852.004	337850.004	124935.193	337850.004
3900.00	34.30900	133364.093	128366.093	122.676771	345075.314	350073.314	128366.093	350073.314
4000.00	34.30900	136794.993	131796.993	123.545400	357386.606	362384.606	131796.993	362384.606
4100.00	34.30900	140225.893	135227.893	124.392579	369783.679	374781.679	135227.893	374781.679
4200.00	34.30900	143656.793	138658.793	125.219341	382264.441	387262.441	138658.793	387262.441
4300.00	34.30900	147087.693	142089.693	126.026649	394826.899	399824.899	142089.693	399824.899
4400.00	34.30900	150518.593	145520.593	126.815397	407469.152	412467.152	145520.593	412467.152
4500.00	34.30900	153949.493	148951.493	127.586418	420189.387	425187.387	148951.493	425187.387
4600.00	34.30900	157380.393	152382.393	128.340492	432985.871	437983.871	152382.393	437983.871
4700.00	34.30900	160811.293	155813.293	129.078349	445856.945	450854.945	155813.293	450854.945
4800.00	34.30900	164242.193	159244.193	129.800670	458801.023	463799.023	159244.193	463799.023
4900.00	34.30900	167673.093	162675.093	130.508097	471816.583	476814.583	162675.093	476814.583
5000.00	34.30900	171103.993	166105.993	131.201232	484902.166	489900.166	166105.993	489900.166
5100.00	34.30900	174534.893	169536.893	131.880640	498056.372	503054.372	169536.893	503054.372
5200.00	34.30900	177965.793	172967.793	132.546855	511277.854	516275.854	172967.793	516275.854
5300.00	34.30900	181396.693	176398.693	133.200380	524565.320	529563.320	176398.693	529563.320
5400.00	34.30900	184827.593	179829.593	133.841688	537917.523	542915.523	179829.593	542915.523
5500.00	34.30900	188258.493	183260.493	134.471229	551333.265	556331.265	183260.493	556331.265
5600.00	34.30900	191689.393	186691.393	135.089426	564811.391	569809.391	186691.393	569809.391
5700.00	34.30900	195120.293	190122.293	135.696680	578350.786	583348.786	190122.293	583348.786
5800.00	34.30900	198551.193	193553.193	136.293374	591950.375	596948.375	193553.193	596948.375
5900.00	34.30900	201982.093	196984.093	136.879867	605609.120	610607.120	196984.093	610607.120
6000.00	34.30900	205412.993	200414.993	137.456502	619326.020	624324.020	200414.993	624324.020

ORIGINAL Mg(cr) Mg(l)

EFDA	MG15	CODA89	HQ/R	-601.1178MP	923.0000NT	70.0000
25.00	0.024054	0.476276	0.005532	50.00	0.190029	0.063022
75.00	0.476276	0.194600	0.194600	100.00	0.772144	0.371038
150.00	1.253231	0.780563	0.780563	200.00	1.592998	1.190449
250.00	1.837751	1.573635	1.573635	298.15	2.016159	1.913237
360.00	2.022168	1.925750	1.925750	350.00	2.166952	2.248822
400.00	2.284861	2.546091	2.546091	450.00	2.384052	2.820945
500.00	2.469418	3.076670	3.076670	600.00	2.612501	3.540116
700.00	2.732744	3.952076	3.952076	800.00	2.840366	4.324097
900.00	2.941578	4.664523	4.664523	923.00	2.964338	4.759038
923.00	4.068935	4.739038	4.739038	1000.00	4.073360	5.065245
1100.00	4.078182	5.453712	5.453712	1200.00	4.082200	5.808737
1300.00	4.085600	6.135625	6.135625	1400.00	4.088515	6.438510
1500.00	4.091040	6.720677	6.720677	1600.00	4.093250	6.984778
1700.00	4.095200	7.232990	7.232990	1800.00	4.096934	7.467115
1900.00	4.098485	7.688667	7.688667	2000.00	4.099880	7.898928
2100.00	4.101143	8.098993	8.098993	2200.00	4.102291	8.289805
2300.00	4.103340	8.472183	8.472183	2400.00	4.104300	8.646840
2500.00	4.105184	8.814404	8.814404	2600.00	4.106000	8.975428
2700.00	4.106756	9.130404	9.130404	2800.00	4.107458	9.279770
2900.00	4.108111	9.423918	9.423918	3000.00	4.108720	9.563199
3100.00	4.109291	9.697933	9.697933	3200.00	4.109826	9.828406
3300.00	4.110328	9.954880	9.954880	3400.00	4.110801	10.077593
3500.00	4.111246	10.196761	10.196761	3600.00	4.111667	10.312585
3700.00	4.112065	10.425246	10.425246	3800.00	4.112443	10.534912
3900.00	4.112801	10.641740	10.641740	4000.00	4.113141	10.745871
4100.00	4.113464	10.847439	10.847439	4200.00	4.113772	10.946567
4300.00	4.114066	11.043370	11.043370	4400.00	4.114346	11.137953
4500.00	4.114614	11.230418	11.230418	4600.00	4.114870	11.320855
4700.00	4.115115	11.409353	11.409353	4800.00	4.115351	11.495993
4900.00	4.115576	11.580851	11.580851	5000.00	4.115793	11.663999
5100.00	4.116001	11.745504	11.745504	5200.00	4.116201	11.825431
5300.00	4.116393	11.903839	11.903839	5400.00	4.116578	11.980785
5500.00	4.116757	12.056322	12.056322	5600.00	4.116929	12.130502
5700.00	4.117095	12.203371	12.203371	5800.00	4.117256	12.274976
5900.00	4.117411	12.345359	12.345359	6000.00	4.117561	12.414562

ORIGINAL Mg(cr) Mg(l)

COEFFICIENTS		Mg(cr)		Mg(l)		Mg(l)		Mg(l)	
ASSIGNED H AT		0 K = -4998.000 J/MOLE							
T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL	
200.00	22.72353	2648.833	-2349.167	23.142628	1979.693	6977.693	-2349.167	6977.693	
298.15	24.86900	4998.000	0.000	32.671000	4742.859	9740.859	0.000	9740.859	
400.00	26.14427	7599.529	2601.529	40.168068	8467.698	13465.698	2601.529	13465.698	
600.00	28.18367	13033.106	8035.106	51.156060	17660.530	22658.530	8035.106	22658.530	
800.00	30.50630	18893.414	13895.414	59.569660	28762.314	33760.314	13895.414	33760.314	
923.00	32.23862	22749.508	17751.508	64.050361	36368.975	41366.975	17751.508	41366.975	
923.00	34.30900	31226.508	26228.508	73.234543	38368.975	41366.975	26228.508	41366.975	
1000.00	34.30900	33868.301	28870.301	75.983588	42115.287	47113.287	28870.301	47113.287	
1200.00	34.30900	40730.101	35732.101	82.238858	57956.529	62954.529	35732.101	62954.529	
1400.00	34.30900	47591.901	42593.901	87.527614	74946.758	79944.758	42593.901	79944.758	
1600.00	34.30900	54453.701	49455.701	92.108942	92920.607	97918.607	49455.701	97918.607	
1800.00	34.30900	61315.501	56317.501	96.149960	111754.428	116752.428	56317.501	116752.428	
2000.00	34.30900	68177.301	63179.301	99.764774	131352.248	136350.248	63179.301	136350.248	
2200.00	34.30900	75039.101	70041.101	103.034771	151637.396	156635.396	70041.101	156635.396	
2400.00	34.30900	81900.901	76902.901	106.020045	172547.206	177545.206	76902.901	177545.206	
2600.00	34.30900	88762.701	83764.701	108.766230	194029.497	199027.497	83764.701	199027.497	
2800.00	34.30900	95624.501	90626.501	111.308800	216040.140	221038.140	90626.501	221038.140	
3000.00	34.30900	102486.301	97488.301	113.675877	238541.329	243539.329	97488.301	243539.329	
3200.00	34.30900	109348.101	104350.101	115.890129	261500.312	266498.312	104350.101	266498.312	
3400.00	34.30900	116209.901	111211.901	117.970099	284888.436	289886.436	111211.901	289886.436	
3600.00	34.30900	123071.701	118073.701	119.951147	308680.428	313678.428	118073.701	313678.428	
3800.00	34.30900	129933.501	124935.501	121.786139	332853.829	337851.829	124935.501	337851.829	
4000.00	34.30900	136795.301	131797.301	123.545961	357388.543	362386.543	131797.301	362386.543	
4200.00	34.30900	143657.101	138659.101	125.219903	382266.491	387264.491	138659.101	387264.491	
4400.00	34.30900	150518.901	145520.901	126.815958	407471.314	412469.314	145520.901	412469.314	
4600.00	34.30900	157380.701	152382.701	128.361053	432988.145	437986.145	152382.701	437986.145	
4800.00	34.30900	164242.501	159244.501	129.801231	458803.409	463801.409	159244.501	463801.409	
5000.00	34.30900	171104.301	166106.301	131.201793	484904.665	489902.665	166106.301	489902.665	
5200.00	34.30900	177966.101	172968.101	132.567417	511280.465	516278.465	172968.101	516278.465	
5400.00	34.30900	184827.901	179829.901	133.842249	537920.246	542918.246	179829.901	542918.246	
5600.00	34.30900	191689.701	186691.701	135.089987	564814.226	569812.226	186691.701	569812.226	
5800.00	34.30900	198551.501	193553.501	136.293935	591953.322	596951.322	193553.501	596951.322	
6000.00	34.30900	205413.301	200415.301	137.457063	619329.079	624327.079	200415.301	624327.079	

COEFFICIENTS Mg(cr) Mg(l)

Example 7 (MgO(g) by Method JANAF with LSQS and LOGK Options)

Problem.—Calculate thermodynamic functions for a species with excited electronic states using method JANAF. Obtain least-squares coefficients and tables with $\Delta_f H_T^\circ$ and $\log_{10} K$ columns.

Except for the missing TEMP records, the LOGK label on the OUTP record, and the data records, the input is similar to that in the previous examples. With no TEMP records, PAC91 uses the default temperature schedule of 100 (100) 6000 K and $T = 298.15$ K. LOGK calls for rounded tables with columns for $\Delta_f H_T^\circ$ and $\log_{10} K$. The data records are for 15 electronic states including the ground state as indicated by the numbers in columns 79 and 80. The excitation energies are given by the T0 numerical values. The remaining labels are defined in table VII. Since no statistical weight was given for the ground state PAC91 assigns a value of 1.

As with the last example, with LSQS on the OUTP record and no LSTSQS records, all the default temperature ranges, constraints, and exponents in equation (11) are set by the program. The default temperature range is 200 to 1000 K for the first interval and 1000 to 6000 K for the second interval. The default constraint temperature is 298.15 K for the first interval and 1000 K for the second interval. This may be seen in the least-squares output table where the errors at 298.15 K are zero and the values of the thermodynamic functions are identical at 1000 K for both the first and second intervals.

Finally, the last two tables in the output are rounded and include columns for $\Delta_f H_T^\circ$ and $\log_{10} K$. One table contains the original data and the other contains data calculated from the least-squares coefficients. Both used the EF data for Mg stored in example 6.

Input. - The input data set for MgO, example 7, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79 80
a NAME	MGO		Magnesium Oxide.	JANAF	Dec.1974, p1	472.	Expl.	7	
MG101	J12/74		HF298	58158.	JOULES				
DATE	JOULES		LOGK		CTAB		LSQS		
OUTP	T	200.	I	100.	T	1000.	I	200.	
CTEM	T	3000.							
METH	JANAF								
DATA	WE	785.1	WEXE	5.18	BE	.5743	ALPHA1	.0050	1
DATA	STATWT	6.	T0	2300.	WE	664.4	WEXE	3.9	2
DATA	BE	.5050	ALPHA1	.004	WE	664.4	WEXE	3.9	2
DATA	STATWT	2.	T0	3503.3	WE	664.4	WEXE	3.9	3
DATA	BE	.5050	ALPHA1	.004	WE	824.1	WEXE	4.8	3
DATA	STATWT	3.	T0	14000.	WE	824.1	WEXE	4.76	4
DATA	BE	.5822	ALPHA1	.0045	WE	824.1	WEXE	5.3	4
DATA	STATWT	1.	T0	20004.	WE	632.5	WEXE	5.3	5
DATA	BE	.5822	ALPHA1	.0045	WE	632.5	WEXE	5.3	5
DATA	STATWT	3.	T0	28000.	WE	632.5	WEXE	5.3	6
DATA	BE	.501	ALPHA1	.0048	WE	632.5	WEXE	5.3	6
DATA	STATWT	6.	T0	29000.	WE	632.5	WEXE	5.3	7
DATA	BE	.501	ALPHA1	.0048	WE	632.5	WEXE	5.3	7
DATA	STATWT	2.	T0	29775.	WE	632.5	WEXE	5.3	8
DATA	BE	.5014	ALPHA1	.0048	WE	632.5	WEXE	5.3	8
DATA	STATWT	3.	T0	30000.	WE	632.5	WEXE	5.3	9
DATA	BE	.501	ALPHA1	.0048	WE	632.4	WEXE	5.2	9
DATA	STATWT	1.	T0	30004.	WE	632.4	WEXE	5.2	10
DATA	BE	.5008	ALPHA1	.0048	WE	632.4	WEXE	5.2	10
DATA	STATWT	1.	T0	37684.	WE	632.4	WEXE	5.2	11
DATA	BE	.5273	ALPHA1	.0048	WE	710.	WEXE	5.	11
DATA	STATWT	6.	T0	37000.	WE	710.	WEXE	5.	12
DATA	BE	.5615	ALPHA1	.005	WE	710.	WEXE	5.	12
DATA	STATWT	2.	T0	37879.	WE	710.	WEXE	5.	13
DATA	BE	.5615	ALPHA1	.005	WE	790.	WEXE	5.	13
DATA	STATWT	6.	T0	39000.	WE	790.	WEXE	5.	14
DATA	BE	.5249	ALPHA1	.005	WE	790.	WEXE	5.	14
DATA	STATWT	2.	T0	39868.	WE	790.	WEXE	5.	15
DATA	BE	.5249	ALPHA1	.005					15
FINISH									

^aAll alphanumeric characters.

Listed output. - Listed output for MgO, example 7, is as follows:

```

NAME  MGO                      Magnesium Oxide.  JANAF Dec.1974, p1472.      Expl. 7
MG101                      HF298      58158.  JOULES

DATE  J12/74

OUTP  JOULES                      LOGK                      CTAB                      LSQS
CTEM  T      200.  I      100.  T      1000.  I      200.
CTEM  T      3000.

METH  JANAF
MOLECULAR WT.= 40.30440

DATA  WE      785.1  WEXE      5.18  BE      .5743  ALPHA1  .0050  1
DATA  STATWT    6.  T0      2300.  WE      664.4  WEXE      3.9  2
DATA  BE      .5050  ALPHA1      .004  2
DATA  STATWT    2.  T0      3503.3  WE      664.4  WEXE      3.9  3
DATA  BE      .5050  ALPHA1      .004  3
DATA  STATWT    3.  T0      14000.  WE      824.1  WEXE      4.8  4
DATA  BE      .5822  ALPHA1      .0045  4
DATA  STATWT    1.  T0      20004.  WE      824.1  WEXE      4.76  5
DATA  BE      .5822  ALPHA1      .0045  5
DATA  STATWT    3.  T0      28000.  WE      632.5  WEXE      5.3  6
DATA  BE      .501  ALPHA1      .0048  6
DATA  STATWT    6.  T0      29000.  WE      632.5  WEXE      5.3  7
DATA  BE      .501  ALPHA1      .0048  7
DATA  STATWT    2.  T0      29775.  WE      632.5  WEXE      5.3  8
DATA  BE      .5014  ALPHA1      .0048  8
DATA  STATWT    3.  T0      30000.  WE      632.5  WEXE      5.3  9
DATA  BE      .501  ALPHA1      .0048  9

BAR  MGO

DATA  STATWT    1.  T0      30004.  WE      632.4  WEXE      5.2  10
DATA  BE      .5008  ALPHA1      .0048  10
DATA  STATWT    1.  T0      37684.  WE      632.4  WEXE      5.2  11
DATA  BE      .5273  ALPHA1      .0048  11
DATA  STATWT    6.  T0      37000.  WE      710.  WEXE      5.  12
DATA  BE      .5615  ALPHA1      .005  12
DATA  STATWT    2.  T0      37879.  WE      710.  WEXE      5.  13
DATA  BE      .5615  ALPHA1      .005  13
DATA  STATWT    6.  T0      39000.  WE      790.  WEXE      5.  14
DATA  BE      .5249  ALPHA1      .005  14
DATA  STATWT    2.  T0      39868.  WE      790.  WEXE      5.  15
DATA  BE      .5249  ALPHA1      .005  15

FINISH

BAR  MGO

```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
200.00	3.6222350	3.6230253	3.5211248	3.5245108	24.1596692	24.1625724	20.6385444	20.6380617
298.15	-0.0007903	-0.0002182	-0.0033859	-0.0009616	-0.0002903	-0.0001202	0.0004827	0.0000234
300.00	3.8695880	3.8695880	3.5939207	3.5939207	25.6505882	25.6505882	22.0566675	22.0566675
400.00	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
500.00	3.8745991	3.8746711	3.5956373	3.5956363	25.6745422	25.6745402	22.0789049	22.0789039
600.00	-0.0000719	-0.0000186	0.0000010	0.0000003	0.0000020	0.0000000	0.0000010	0.0000000
700.00	4.1834225	4.1803965	3.7020302	3.7017295	26.8292628	26.8289409	23.1272326	23.1272114
800.00	0.0025260	0.0006038	0.0003007	0.0000812	0.0003219	0.0000120	0.0000212	0.0000009
900.00	4.6225831	4.6241862	3.8397236	3.8393366	27.8071580	27.8066531	23.9674344	23.9673165
1000.00	-0.0016032	-0.0003468	0.0003869	0.0001008	0.0005049	0.0000182	0.0001179	0.0000049
1100.00	5.1811418	5.1827699	4.0157194	4.0157747	28.6981979	28.6981068	24.6824784	24.6823321
1200.00	-0.0016281	-0.0003142	-0.0000553	-0.0000138	0.0000911	0.0000032	0.0001463	0.0000059
1300.00	5.7472747	5.7457533	4.2233515	4.2233775	29.5401461	29.5400372	25.3167947	25.3166597
1400.00	0.0015214	0.0002647	-0.0000260	-0.0000069	0.0001089	0.0000037	0.0001349	0.0000053
1500.00	6.2013558	6.2012364	4.4438496	4.4437241	30.3389662	30.3386969	25.8951166	25.8949723
1600.00	0.0001194	0.0000192	0.0001255	0.0000282	0.0002693	0.0000089	0.0001438	0.0000056
1700.00	6.4815119	6.4823453	4.6563835	4.6563580	31.0873489	31.0871685	26.4309654	26.4308104
1800.00	-0.0008335	-0.0001286	0.0000255	0.0000055	0.0001804	0.0000058	0.0001550	0.0000057
1900.00	6.5903910	6.5901425	4.8456316	4.8455819	31.7772400	31.7770331	26.9316084	26.9314511
2000.00	0.0002485	0.0000377	0.0000497	0.0000103	0.0002070	0.0000065	0.0001573	0.0000058

MAX REL ERR CP/R = 0.000604 TEMP = 400.0
 MAX REL ERR HH/RT = 0.000962 TEMP = 200.0
 MAX REL ERR S/R = 0.000120 TEMP = 200.0
 MAX REL ERR GH/RT = 0.000023 TEMP = 200.0
 MAX ERR CP/R = 0.002526 TEMP = 400.0
 MAX ERR HH/RT = 0.003386 TEMP = 200.0
 MAX ERR S/R = 0.002903 TEMP = 200.0
 MAX ERR GH/RT = 0.000483 TEMP = 200.0
 CP/R = 3.7782309e+05T**2.0 -6.0817323e+03T**1.0
 -1.4549526e-07T**3.0 4.0351763e-11T**4.0
 (H-H0)/R CONSTANT = 0.28401570e+05, H/R CONSTANT = 0.34326805e+05, S/R CONSTANT = -0.20182814e+03

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
1000.00	6.5903910	6.5901425	4.8456316	4.8455819	31.7772400	31.7770331	26.9316084	26.9314511
1100.00	0.0002485	0.0000377	0.0000497	0.0000103	0.0002070	0.0000065	0.0001573	0.0000058
1200.00	6.5678619	6.5718199	5.0043032	5.0043038	32.4051630	32.4053238	27.4011327	27.4009849
1300.00	-0.0039580	-0.0006026	-0.0003086	-0.0000617	-0.0001608	-0.0000050	0.0001478	0.0000054
1400.00	6.4621804	6.4608150	5.1303682	5.1307452	32.9725516	32.9728243	27.8421834	27.8420694
1500.00	0.0013655	0.0002113	-0.0003867	-0.0000754	-0.0002727	-0.0000083	0.0001140	0.0000041
1600.00	6.3137782	6.3101469	5.2272787	5.2274152	33.4841208	33.4841648	28.2568421	28.2567496
1700.00	0.0036313	0.0005751	-0.0001365	-0.0000261	-0.0000441	-0.0000013	0.0000925	0.0000033
1800.00	6.1506734	6.1480945	5.2990894	5.2989786	33.9460831	33.9458801	28.6469937	28.6469015
1900.00	0.0025789	0.0004193	0.0001108	0.0000209	0.0002030	0.0000060	0.0000922	0.0000032
2000.00	5.9898031	5.9895149	5.3504543	5.3502549	34.3649022	34.3646003	29.0144479	29.0143453
2100.00	0.0002882	0.0000481	0.0001994	0.0000373	0.0003019	0.0000088	0.0001075	0.0000035
2200.00	5.8401423	5.8418349	5.3856640	5.3855255	34.7466245	34.7463701	29.3609605	29.3608446
2300.00	-0.0016926	-0.0002898	0.0001385	0.0000257	0.0002544	0.0000073	0.0001160	0.0000039
2400.00	5.7056142	5.7083273	5.4083633	5.4083637	35.0965646	35.0964475	29.6882013	29.6880803
2500.00	-0.0027131	-0.0004755	-0.0000039	-0.0000007	0.0001171	0.0000033	0.0001210	0.0000041
2600.00	5.5871912	5.5899504	5.4215136	5.4216733	35.4193034	35.4193034	29.9977462	29.9976301
2700.00	-0.0027591	-0.0004938	-0.0001598	-0.0000295	-0.0000437	-0.0000012	0.0001161	0.0000039
2800.00	5.4843087	5.4863980	5.4274607	5.4277447	35.7185218	35.7186974	30.2910611	30.2909557
2900.00	-0.0020893	-0.0003810	-0.0002810	-0.0000518	-0.0001756	-0.0000049	0.0001054	0.0000035
3000.00	5.3956638	5.3967080	5.4280310	5.4283737	35.9975185	35.9977755	30.5694876	30.5693985
3100.00	-0.0010442	-0.0001935	-0.0003660	-0.0000667	-0.0002570	-0.0000071	0.0000890	0.0000032
3200.00	5.3196868	5.3196147	5.4246340	5.4249861	36.2588887	36.2591679	30.8342547	30.8341818
3300.00	0.0000721	0.0000135	-0.0003521	-0.0000649	-0.0002792	-0.0000077	0.0000729	0.0000024
3400.00	5.2548048	5.2537533	5.4183512	5.4186597	36.5048226	36.5050755	31.0864715	31.0864159
3500.00	0.0010516	0.0002001	-0.0003085	-0.0000569	-0.0002529	-0.0000066	0.0000566	0.0000023
3600.00	5.1995323	5.1977745	5.4100046	5.4102395	36.7371545	36.7373450	31.3271499	31.3271055
3700.00	0.0017577	0.0003381	-0.0002348	-0.0000405	-0.0001905	-0.0000052	0.0000444	0.0000021
3800.00	5.1525519	5.1504084	5.4002295	5.4003721	36.9574251	36.9575310	31.5571957	31.5571589
3900.00	0.0021435	0.0004160	-0.0001427	-0.0000264	-0.0001059	-0.0000029	0.0000368	0.0000021
4000.00	5.1127103	5.1104947	5.3895044	5.3895523	37.1669325	37.1669483	31.7774281	31.7773961
4100.00	0.0022156	0.0004333	-0.0000479	-0.0000089	-0.0000158	-0.0000004	0.0000320	0.0000010
4200.00	5.0790145	5.0769959	5.3781910	5.3781561	37.3667814	37.3667136	31.9885904	31.9885575
4300.00	0.0020186	0.0003974	0.0000349	0.0000065	0.0000678	0.0000018	0.0000329	0.0000010
4400.00	5.0506094	5.0489979	5.3665705	5.3664678	37.5579187	37.5577801	32.1913482	32.1913122
4500.00	0.0016115	0.0003191	0.0001027	0.0000138	0.0000386	0.0000037	0.0000360	0.0000011
4600.00	5.0267711	5.0257060	5.3548470	5.3547008	37.7411535	37.7409661	32.3863065	32.3862653
4700.00	0.0010651	0.0002119	0.0001462	0.0000273	0.0001874	0.0000050	0.0000412	0.0000013
4800.00	5.0068916	5.0064360	5.3431807	5.3430132	37.9171920	37.9169778	32.5740114	32.5739646
4900.00	0.0004556	0.0000910	0.0001675	0.0000313	0.0002143	0.0000057	0.0000468	0.0000014
5000.00	4.9904468	4.9906046	5.3316879	5.3315213	38.0866465	38.0864279	32.7549586	32.7549063
5100.00	-0.0001577	-0.0000316	0.0001667	0.0000333	0.0002186	0.0000057	0.0000519	0.0000016
5200.00	4.9770043	4.9777187	5.3204565	5.3203088	38.2500543	38.2498514	32.9295978	32.9295426
5300.00	-0.0007144	-0.0001435	0.0001477	0.0000278	0.0002030	0.0000053	0.0000553	0.0000017
5400.00	4.9661894	4.9673659	5.3095484	5.3094350	38.4078906	38.4077178	33.0983422	33.0982828
5500.00	-0.0011766	-0.0002369	0.0001134	0.0000214	0.0001728	0.0000045	0.0000594	0.0000018
5600.00	4.9576880	4.9592038	5.2990103	5.2989404	38.5605739	38.5604417	33.2615636	33.2615013
5700.00	-0.0015158	-0.0003057	0.0000698	0.0000132	0.0001322	0.0000034	0.0000624	0.0000019
5800.00	4.9512419	4.9529514	5.2888708	5.2888519	38.7084752	38.7083913	33.4196044	33.4195395
5900.00	-0.0017095	-0.0003453	0.0000190	0.0000036	0.0000839	0.0000022	0.0000649	0.0000019
6000.00	4.9466200	4.9483804	5.2791548	5.2791856	38.8519289	38.8518954	33.5727741	33.5727098
6100.00	-0.0017604	-0.0003559	-0.0000308	-0.0000050	0.0000335	0.0000009	0.0000643	0.0000019
6200.00	4.9436377	4.9453076	5.2698727	5.2699506	38.9912333	38.9912492	33.7213606	33.7212986
6300.00	-0.0016699	-0.0003378	-0.0000780	-0.0000148	-0.0000159	-0.0000004	0.0000620	0.0000018
6400.00	4.9421373	4.9435882	5.2610321	5.2611504	39.1266625	39.1267192	33.8656304	33.8655683
6500.00	-0.0014508	-0.0002936	-0.0001182	-0.0000225	-0.0000567	-0.0000014	0.0000615	0.0000013
6600.00	4.9419801	4.9431088	5.2526350	5.2528745	39.2584538	39.2584700	34.0052188	34.0051675
6700.00	-0.0011287	-0.0002284	-0.0001495	-0.0000285	-0.0000932	-0.0000024	0.0000563	0.0000017
6800.00	4.9430465	4.9437827	5.2446814	5.2448504	39.3869366	39.3869530	34.1421553	34.1421072
6900.00	-0.0007362	-0.0001489	-0.0001690	-0.0000322	-0.0001163	-0.0000030	0.0000527	0.0000015
7000.00	4.9452504	4.9455440	5.2371664	5.2373435	39.5120094	39.5121387	34.2748430	34.2747952
7100.00	-0.0002937	-0.0000594	-0.0001771	-0.0000338	-0.0001293	-0.0000033	0.0000478	0.0000014

BAR MGO

4100.00	4.9485103	4.9483438	5.2300825	5.2302585	39.6341581	39.6342894	34.4040756	34.4040309
	0.0001665	0.0000336	-0.0001760	-0.0000337	-0.0001313	-0.0000033	0.0000447	0.0000013
4200.00	4.9527482	4.9521454	5.2234278	5.2235896	39.7534544	39.7535760	34.5300266	34.5299865
	0.0006028	0.0001217	-0.0001618	-0.0000310	-0.0001216	-0.0000031	0.0000402	0.0000012
4300.00	4.9579160	4.9569212	5.2171907	5.2173306	39.8700514	39.8701565	34.6528606	34.6528260
	0.0009947	0.0002006	-0.0001398	-0.0000268	-0.0001052	-0.0000026	0.0000347	0.0000010
4400.00	4.9639549	4.9626494	5.2113657	5.2114755	39.9841010	39.9841776	34.7727353	34.7727021
	0.0013055	0.0002630	-0.0001098	-0.0000211	-0.0000766	-0.0000019	0.0000332	0.0000010
4500.00	4.9708240	4.9693107	5.2059412	5.2060183	40.0957288	40.0957753	34.8897876	34.8897570
	0.0015133	0.0003044	-0.0000771	-0.0000148	-0.0000465	-0.0000012	0.0000306	0.0000007
4600.00	4.9784954	4.9768861	5.2009125	5.2009532	40.2050650	40.2050766	35.0041526	35.0041234
	0.0016093	0.0003232	-0.0000407	-0.0000078	-0.0000116	-0.0000003	0.0000292	0.0000003
4700.00	4.9869234	4.9853543	5.1962681	5.1962743	40.3122230	40.3121997	35.1159549	35.1159253
	0.0015691	0.0003146	-0.0000063	-0.0000012	0.0000233	0.0000006	0.0000295	0.0000003
4800.00	4.9960817	4.9946897	5.1920023	5.1919759	40.4173114	40.4172548	35.2253091	35.2252789
	0.0013919	0.0002786	0.0000264	0.0000051	0.0000566	0.0000014	0.0000302	0.0000009
4900.00	5.0059449	5.0048605	5.1881027	5.1880521	40.5204267	40.5203449	35.3323240	35.3322928
	0.0010844	0.0002166	0.0000506	0.0000098	0.0000819	0.0000020	0.0000312	0.0000009
5000.00	5.0164955	5.0158267	5.1845655	5.1844966	40.6216671	40.6215657	35.4371015	35.4370691
	0.0006687	0.0001333	0.0000689	0.0000133	0.0001014	0.0000025	0.0000324	0.0000007
5100.00	5.0277036	5.0275392	5.1813784	5.1813030	40.7211166	40.7210066	35.5397382	35.5397036
	0.0001644	0.0000327	0.0000753	0.0000145	0.0001100	0.0000027	0.0000346	0.0000010
5200.00	5.0395491	5.0399376	5.1785355	5.1784642	40.8185581	40.8187508	35.6403226	35.6402866
	-0.0003886	-0.0000771	0.0000713	0.0000138	0.0001073	0.0000026	0.0000360	0.0000010
5300.00	5.0520177	5.0529496	5.1760302	5.1759723	40.9149710	40.9148751	35.7389408	35.7389028
	-0.0009319	-0.0001845	0.0000578	0.0000112	0.0000959	0.0000023	0.0000381	0.0000011
5400.00	5.0650799	5.0664895	5.1738529	5.1738188	41.0094509	41.0094509	35.8356694	35.8356321
	-0.0014095	-0.0002783	0.0000341	0.0000066	0.0000714	0.0000017	0.0000373	0.0000010
5500.00	5.0787232	5.0804571	5.1719980	5.1719937	41.1025859	41.1025438	35.9305878	35.9305501
	-0.0017339	-0.0003414	0.0000043	0.0000008	0.0000421	0.0000010	0.0000378	0.0000011
5600.00	5.0929281	5.0947372	5.1704597	5.1704863	41.1942139	41.1942139	36.0237651	36.0237277
	-0.0018091	-0.0003552	-0.0000265	-0.0000051	0.0000109	0.0000003	0.0000374	0.0000010
5700.00	5.1076726	5.1091983	5.1692276	5.1692276	41.2844981	41.2845161	36.1152705	36.1152320
	-0.0015257	-0.0002987	-0.0000564	-0.0000109	-0.0000180	-0.0000004	0.0000385	0.0000011
5800.00	5.1229418	5.1236919	5.1682978	5.1683731	41.3734610	41.3734997	36.2051633	36.2051266
	-0.0007501	-0.0001464	-0.0000753	-0.0000146	-0.0000386	-0.0000009	0.0000367	0.0000010
5900.00	5.1387049	5.1380521	5.1676607	5.1677378	41.4611648	41.4612090	36.2935041	36.2934712
	0.0006528	0.0001270	-0.0000771	-0.0000149	-0.0000442	-0.0000011	0.0000329	0.0000009
6000.00	5.1549559	5.1520945	5.1673117	5.1673606	41.5476667	41.5476831	36.3803551	36.3803225
	0.0028614	0.0005551	-0.0000490	-0.0000095	-0.0000164	-0.0000004	0.0000326	0.0000009
MAX REL ERR CP/R	= 0.000603	TEMP = 1100.	AVER REL ERR CP/R	= 0.000259	REL LST SQ ERR CP/R	= 0.000298		
MAX REL ERR HH/RT	= 0.000075	TEMP = 1200.	AVER REL ERR HH/RT	= 0.000023	REL LST SQ ERR HH/RT	= 0.000029		
MAX REL ERR S/R	= 0.000009	TEMP = 1500.	AVER REL ERR S/R	= 0.000003	REL LST SQ ERR S/R	= 0.000004		
MAX REL ERR GH/RT	= 0.000006	TEMP = 1000.	AVER REL ERR GH/RT	= 0.000002	REL LST SQ ERR GH/RT	= 0.000002		
MAX ERR CP/R	= 0.003958	TEMP = 1100.	AVER ERR CP/R	= 0.001377	LST SQ ERR CP/R	= 0.001623		
MAX ERR HH/RT	= 0.000387	TEMP = 1200.	AVER ERR HH/RT	= 0.000123	LST SQ ERR HH/RT	= 0.000155		
MAX ERR S/R	= 0.000302	TEMP = 1500.	AVER ERR S/R	= 0.000119	LST SQ ERR S/R	= 0.000144		
MAX ERR GH/RT	= 0.000157	TEMP = 1000.	AVER ERR GH/RT	= 0.000059	LST SQ ERR GH/RT	= 0.000067		
CP/R	= -1.3876702e+07T**2.0	3.3903403e+04T**1.0	-2.1906072e+01T**0.0	1.0456393e-02T**1.0	-2.2225473e-06T**2.0			
	2.4662915e-10T**3.0	-1.0961026e-14T**4.0						
(H-H0)/R	CONSTANT = -0.22586827e+06,	H/R	CONSTANT = -0.21994504e+06,	S/R	CONSTANT = 0.20063928e+03			

BAR MGO

TAHERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

MGD	Magnesium Oxide.	JANAF Dec.1974, p1472.	Expt. 7
2 J12/74 MG	1.000 1.00 0.00 0.00 0.00 0	40.30440	58158.000
200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0			8909.226
3.77823092d+05 -6.08173235d+03 4.16158227d+01 -1.18519891d-01 1.94341613d-04			
-1.45495255d-07 4.03517625d-11 0.00000000d+00 3.43248026d+04 -2.01828144d+02			
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0			8909.226
-1.38767024d+07 3.39034027d+04 -2.19060721d+01 1.04563934d-02 -2.22254732d-06			
2.46629150d-10 -1.09610259d-14 0.00000000d+00 -2.19945038d+05 2.00639280d+02			

ORIGINAL BAR MGO

ORIGINAL		MGD						
T DEG-K	CP J/MOL-KG	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K	
0	-----	-8.909	-----	-----	49.249	58.587	-----	
100	29.125	-6.001	180.487	240.496	52.157	59.403	-26.6232	
200	30.117	-3.054	200.876	216.146	55.104	58.887	-11.1490	
298.15	32.174	0.000	213.272	213.272	58.158	58.158	-6.1132	
300	32.215	0.060	213.471	213.273	58.218	58.144	-6.0503	
400	34.783	3.403	223.072	214.565	61.561	57.447	-3.5336	
500	38.435	7.053	231.203	217.096	65.211	56.901	-2.0403	
600	43.079	11.124	238.611	220.071	69.282	56.624	-1.0523	
700	47.786	15.671	245.612	223.224	73.829	56.672	-0.3482	
800	51.561	20.650	252.254	226.442	78.808	56.993	0.1817	
900	55.891	25.935	258.476	229.660	84.093	57.457	0.5968	
* 1000	54.796	31.380	264.212	232.832	89.538	49.314	0.8943	
1100	54.609	36.857	269.433	235.926	95.015	49.605	1.1292	
1200	53.730	42.279	274.151	238.918	100.437	49.821	1.3259	
1300	52.496	47.592	278.404	241.795	105.750	49.910	1.4929	
1400	51.140	52.774	282.245	244.549	110.932	49.854	1.6361	
1500	49.802	57.820	285.727	247.180	115.978	49.648	1.7599	
1600	48.558	62.737	288.901	249.690	120.895	49.299	1.8676	
1700	47.439	67.536	291.811	252.084	125.694	48.820	1.9618	
1800	46.455	72.230	294.494	254.366	130.388	48.223	2.0447	
1900	45.599	76.831	296.982	256.544	134.989	47.523	2.1178	
2000	44.862	81.354	299.302	258.625	139.512	46.731	2.1826	
2100	44.231	85.807	301.475	260.614	143.965	45.859	2.2402	
2200	43.691	90.203	303.520	262.518	148.361	44.917	2.2915	
2300	43.232	94.548	305.451	264.343	152.706	43.913	2.3374	
2400	42.841	98.851	307.283	266.095	157.009	42.856	2.3785	
2500	42.510	103.118	309.025	267.777	161.276	41.752	2.4153	
2600	42.230	107.355	310.686	269.396	165.513	40.606	2.4484	
2700	41.993	111.566	312.276	270.955	169.724	39.423	2.4782	
2800	41.795	115.755	313.799	272.458	173.913	38.207	2.5050	
2900	41.630	119.926	315.263	273.909	178.084	36.963	2.5292	
3000	41.493	124.082	316.672	275.311	182.240	35.694	2.5510	
3100	41.381	128.225	318.030	276.667	186.383	34.403	2.5707	
3200	41.291	132.359	319.343	277.981	190.517	33.091	2.5885	
3300	41.221	136.484	320.612	279.253	194.642	31.763	2.6045	
3400	41.167	140.604	321.842	280.488	198.762	30.418	2.6190	
3500	41.129	144.718	323.035	281.687	202.876	29.061	2.6321	
3600	41.104	148.830	324.193	282.851	206.988	27.692	2.6438	
3700	41.091	152.940	325.319	283.984	211.098	26.312	2.6544	
3800	41.090	157.049	326.415	285.086	215.207	24.925	2.6639	
3900	41.099	161.158	327.482	286.160	219.316	23.529	2.6725	
4000	41.117	165.269	328.523	287.206	223.427	22.127	2.6801	
4100	41.144	169.382	329.539	288.226	227.540	20.720	2.6869	
4200	41.180	173.498	330.530	289.221	231.656	19.310	2.6930	
4300	41.223	177.618	331.500	290.195	235.776	17.896	2.6984	
4400	41.273	181.743	332.448	291.143	239.901	16.480	2.7031	
4500	41.330	185.873	333.376	292.071	244.031	15.063	2.7073	
4600	41.394	190.009	334.285	292.979	248.167	13.645	2.7109	
4700	41.464	194.152	335.176	293.868	252.310	12.228	2.7140	
4800	41.540	198.302	336.050	294.737	256.460	10.812	2.7167	
4900	41.622	202.460	336.907	295.589	260.618	9.398	2.7190	
5000	41.710	206.626	337.749	296.424	264.784	7.987	2.7208	
5100	41.803	210.802	338.576	297.242	268.960	6.578	2.7223	
5200	41.901	214.987	339.389	298.045	273.145	5.175	2.7235	
5300	42.005	219.182	340.188	298.833	277.340	3.776	2.7245	
5400	42.114	223.388	340.974	299.606	281.546	2.382	2.7249	
5500	42.227	227.605	341.748	300.365	285.763	0.995	2.7252	
5600	42.345	231.834	342.510	301.111	289.992	-0.386	2.7252	
5700	42.468	236.074	343.260	301.844	294.232	-1.759	2.7251	
5800	42.595	240.328	344.000	302.564	298.486	-3.124	2.7247	
5900	42.726	244.594	344.729	303.273	302.752	-4.480	2.7241	
6000	42.861	248.873	345.448	303.970	307.031	-5.827	2.7233	

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE.
MG-- 923.000

COEFFICIENTS		MGD						
T DEG-K	CP J/MOL-K	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K	
0	-----	-8.909	-----	-----	49.249	58.587	-----	
200	30.124	-3.048	200.900	216.141	55.110	58.893	-11.1492	
298.15	32.174	0.000	213.272	213.272	58.158	58.158	-6.1132	
300	32.216	0.060	213.471	213.273	58.218	58.144	-6.0503	
400	34.762	3.402	223.069	214.564	61.560	57.446	-3.5336	
500	38.448	7.052	231.199	217.095	65.210	56.899	-2.0403	
600	43.092	11.124	238.611	220.070	69.282	56.625	-1.0524	
700	47.773	15.671	245.611	223.223	73.829	56.672	-0.3482	
800	51.560	20.649	252.251	226.441	78.807	56.993	0.1817	
900	55.898	25.935	258.475	229.658	84.093	57.456	0.5967	
* 1000	54.794	31.379	264.210	232.831	89.537	49.314	0.8942	
1200	53.719	42.282	274.153	238.918	100.440	49.824	1.3258	
1400	51.118	52.773	282.243	244.549	110.931	49.853	1.6361	
1600	48.572	62.756	288.899	249.689	120.896	49.297	1.8675	
1800	46.478	72.232	294.494	254.365	130.390	48.226	2.0446	
2000	44.871	81.359	299.304	258.624	139.517	46.737	2.1826	
2200	43.682	90.208	303.522	262.518	148.366	44.922	2.2915	
2400	42.823	98.854	307.284	266.094	157.012	42.859	2.3785	
2600	42.213	107.354	310.686	269.396	165.512	40.605	2.4484	
2800	41.786	115.752	313.798	272.458	173.910	38.204	2.5050	
3000	41.494	124.078	316.670	275.311	182.236	35.690	2.5510	

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE.
MG-- 923.000

COEFFICIENTS BAR MGD

Example 8 ($\text{Na}_2\text{CO}_3(1,2,\ell)$ by Methods READIN and COEF with LSQS and LOGK Options)

Problem.—Calculate thermodynamic properties for a condensed species with more than two phases. Use different methods for processing the data, if needed. Obtain least-squares coefficients and tables with $\Delta_f H_T^\circ$ and $\log_{10} K$ columns.

The species selected for this example is Na_2CO_3 which has three condensed phases—two solid and one liquid. This example illustrates the following features:

(1) The NAME records identify the three phases as $\text{Na}_2\text{CO}_3(1)$, $\text{Na}_2\text{CO}_3(2)$, and $\text{Na}_2\text{CO}_3(\ell)$. These names appear as identification in the least-squares coefficient output.

(2) The data for the two solid phases are processed by METHOD READIN, while the liquid phase is processed by METHOD COEF. The energy unit for input data is in calories as indicated by the CAL label on the METHOD records.

(3) The heat of formation at 298.15 K is specified to be -270.26 kcal/mol by HF298 and KCAL on the formula record.

(4) The OUTP record contains the labels LOGK, JOULES, and LSQS. The LSQS label calls for output tables of functions calculated from least-squares coefficients. Separate sets of coefficients will be generated for each phase. The LOGK label calls for tables of rounded functions including $\Delta_f H_T^\circ$ and $\log_{10} K$. The label JOULES specifies that the unit of energy in the output tables is in joules.

(5) The first METHOD record specifies that the energy unit on the input data records following it is in calories (CAL).

(Note that while the input is in calories the output, as discussed in (4) above, is to be in joules.)

(6) The heat of transition between the first and second phase is given by the value of 165. for the DELTAH label on the second METHOD record. The energy unit is cal/mol (CAL).

(7) No enthalpy or entropy values are given on the first data record for the second phase at the transition temperature of 723.15 K. These values are calculated by the program from the DELTAH value of 165 cal/mol and the enthalpy and entropy values of the first phase at 723.15 K.

(8) The heat of transition of 7090. between phases 2 and 3 (the heat of fusion) is given on the third METHOD record as the DELTAH numerical value. The energy unit is cal/mol (CAL).

(9) On the first data record for the liquid phase, C1 is given as 45.30.

(10) On the second data record for the liquid phase, only the TCOEF label appears. The purpose of the TCOEF label was discussed in the example for $\text{Mg}(\ell)$.

(11) The listed output consists of a table of the input records, a table of least-squares coefficients and errors, and a table of rounded thermodynamic functions. Note that at each transition temperature ($T = 723.15$ and 1123.15 K) values of $-(G-H298)/T$ and LOGK are identical for the two phases. The columns headed DELTA H and LOGK do not contain data for temperatures at 2400 K and higher, inasmuch as the EF data for $\text{Na}(\ell)$ exist only to 2300 K.

Input. - The input data set for $\text{Na}_2\text{CO}_3(1,2,0)$, example 8, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79 80
a	NAME	NA2C03(1)	JANAF	DATA. MARCH 1966.				Expl.	8
a	NAME	NA2C03(2)	JANAF	DATA. MARCH 1966.					
a	NAME	NA2C03(L)	JANAF	DATA. MARCH 1966.					
	NA2C103(S)		HF298	-270.26	KCAL				
	DATE	J 3/66							
	OUTP	LOGK							
	METHOD	READIN	JOULES		LSQS				
			H298H0	4974.	MELTPT	1123.15	CAL		
	T	100.	CP	14.637	S	10.334	H-H2	-4348.	
	T	200.	CP	22.5000	S	23.367	H-H2	-2424.	
	T	298.15	CP	26.530	S	33.173	H-H2	0.0	
	T	300.	CP	26.590	S	33.338	H-H2	49.0	
	T	400.	CP	29.900	S	41.421	H-H2	2867.	
	T	500.	CP	33.990	S	48.520	H-H2	6056.	
	T	600.	CP	39.030	S	55.153	H-H2	9702.	
	T	700.	CP	44.830	S	61.597	H-H2	13890.	
	T	723.15	CP	46.220	S	63.078	H-H2	14944.	
	METHOD	READIN	DELTAH	165.	CAL				
	T	723.15	CP	34.360	S		H-H2		
	T	800.	CP	36.650	S	66.889	H-H2	17837.	
	T	900.	CP	39.730	S	71.383	H-H2	21655.	
	T	1000.	CP	42.830	S	75.729	H-H2	25782.	
	T	1100.	CP	45.900	S	79.956	H-H2	30220.	
	T	1123.15	CP	46.630	S	80.920	H-H2	31291.	
TEMP	T	1123.15	T	1200.	I	200.	T	6000.	
METH	COEF		DELTAH	7090.0	CAL				
	T	1123.15	T	6000.	C1	45.30	E1	0.0	
FINISH	TCOEF								

^aAll alphanumeric characters.

Listed output. - Listed output for $\text{Na}_2\text{CO}_3(1,2,0)$, example, 8, is as follows:

```

NAME HA2CO3(1)      JANAF DATA.  MARCH 1966.      Expl. 8
NAME HA2CO3(2)      JANAF DATA.  MARCH 1966.
NAME HA2CO3(L)      JANAF DATA.  MARCH 1966.
HA2CO3(S)           HF298 -270.26      KCAL
DATE J 3/66
OUTP LOGK           JOULES              LSQS
METHODREADIN        H298H0 4974.      MELTPT 1123.15  CAL
    T    100.      CP    14.637      S    10.334      H-H2  -4348.
    T    200.      CP    22.5000     S    23.367      H-H2  -2424.
    T    298.15    CP    26.530      S    33.173      H-H2   0.0
    T    300.      CP    26.590      S    33.338      H-H2   49.0
    T    400.      CP    29.900      S    41.421      H-H2  2867.
    T    500.      CP    33.990      S    48.520      H-H2  6056.
    T    600.      CP    39.030      S    55.153      H-H2  9702.
    T    700.      CP    44.830      S    61.597      H-H2 13890.
    T    723.15    CP    46.220      S    63.078      H-H2 14944.
METHODREADIN        DELTAH 165.      CAL

LEAST SQUARES

    T    CP/R INPUT    CP/R CALC    HH/RT INPUT    HH/RT CALC    S/R INPUT    S/R CALC    -GH/RT INPUT    -GH/RT CALC
          INPUT-CALC    FRACTION    INPUT-CALC    FRACTION    INPUT-CALC    FRACTION    INPUT-CALC    FRACTION
200.00   11.3223750    11.3218818    6.4160125     6.4142146    11.7586638    11.7561738    5.3426513    5.3419592
          0.0004931     0.0000436     0.0017979     0.0002802     0.0024900     0.0002118     0.0006921     0.0001295
298.15   13.3503381    13.3503381    8.3951021     8.3951021    16.6932065    16.6932065    8.2981043    8.2981043
          0.0000000     0.0000000     0.0000000     0.0000000     0.0000000     0.0000000     0.0000000     0.0000000
300.00   13.3805311    13.3807015    8.4255244     8.4257531    16.7762372    16.7758823    8.3507128    8.3501292
          -0.0001704     -0.0000127    -0.0002287    -0.0000271    0.0003549     0.0000212     0.0005836     0.0000699
400.00   15.0461783    15.0471258    9.8643047     9.8689109    20.8437375    20.8491163    10.9794328    10.9802053
          -0.0009475     -0.0000630    -0.0046062    -0.0004670    -0.0053787    -0.0002581    -0.0007725    -0.0000704
500.00   17.1043345    17.1006858    11.1009596    11.1014685    24.4160726    24.4179923    13.3151130    13.3165238
          0.0036487     0.0002133    -0.0005089    -0.0000458    -0.0019197    -0.0000786    -0.0014108    -0.0001060
600.00   19.6405465    19.6447778    12.3086796    12.3071219    27.7539088    27.7538865    15.4452291    15.4467646
          -0.0042313    -0.0002154    0.0015578     0.0001266     0.0000223     0.0000008    -0.0015355    -0.0000994
700.00   22.5592031    22.5547150    13.5609703    13.5599048    30.9966370    30.9970958    17.4356667    17.4371910
          0.0044881     0.0001989     0.0010655     0.0000786    -0.0004588    -0.0000148    -0.0015243    -0.0000874
723.15   23.2586743    23.2615218    13.8602912    13.8591431    31.7419008    31.7423558    17.8816097    17.8832127
          -0.0028475    -0.0001224     0.0011481     0.0000828    -0.0004549    -0.0000143    -0.0016030    -0.0000896
MAX REL ERR CP/R = 0.000215 TEMP = 600.      AVER REL ERR CP/R = 0.000109 REL LST SQ ERR CP/R = 0.000138
MAX REL ERR HH/RT = 0.000467 TEMP = 400.      AVER REL ERR HH/RT = 0.000139 REL LST SQ ERR HH/RT = 0.000203
MAX REL ERR S/R = 0.000258 TEMP = 400.      AVER REL ERR S/R = 0.000075 REL LST SQ ERR S/R = 0.000122
MAX REL ERR GH/RT = 0.000130 TEMP = 200.      AVER REL ERR GH/RT = 0.000082 REL LST SQ ERR GH/RT = 0.000089
MAX ERR CP/R = 0.004488 TEMP = 700.      AVER ERR CP/R = 0.002103 LST SQ ERR CP/R = 0.002753
MAX ERR HH/RT = 0.004606 TEMP = 400.      AVER ERR HH/RT = 0.001364 LST SQ ERR HH/RT = 0.001925
MAX ERR S/R = 0.005379 TEMP = 400.      AVER ERR S/R = 0.001385 LST SQ ERR S/R = 0.002218
MAX ERR GH/RT = 0.001603 TEMP = 723.      AVER ERR GH/RT = 0.001015 LST SQ ERR GH/RT = 0.001154
CP/R = 2.7690834e+051**2.0 -6.2925704e+051**1.0 5.4857058e+011** 0.0 -1.3550634e-011** 1.0 2.3061993e-041** 2.0
      -1.4673680e-071** 3.0 3.4582744e-111** 4.0
(H-H0)/R CONSTANT = 0.27187630e+05, H/R CONSTANT =-0.11131471e+06, S/R CONSTANT =-0.28402909e+03

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -
HA2CO3(1)      JANAF DATA.  MARCH 1966.      Expl. 8
1 J 3/66 HA 2.00C 1.000 3.00 0.00 0.00 1 105.98874 -1130767.840
200.000 723.150 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20811.216
2.76908339d+05 -6.29257045d+03 5.48570580d+01 -1.35506338d-01 2.30619932d-04
-1.46736800d-07 3.45827436d-11 0.00000000d+00 -1.11314706d+05 -2.84029093d+02
    T    723.15    CP    34.360      S              H-H2
    T    800.      CP    36.650      S    66.889      H-H2 17837.
    T    900.      CP    39.730      S    71.383      H-H2 21655.
                                HA2CO3(1)      HA2CO3(2)      HA2CO3(L)
    T    1000.     CP    42.830      S    75.729      H-H2 25782.
    T    1100.     CP    45.900      S    79.956      H-H2 30220.
    T    1123.15   CP    46.630      S    80.920      H-H2 31291.
TEMP T 1123.15    T 1200.      I 200.      T 6000.
METH COEF        DELTAH7090.0      CAL

                                HA2CO3(1)      HA2CO3(2)      HA2CO3(L)

```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
723.15	17.2905246	17.2905246	13.9751093	13.9739612	31.8567190	31.8571739	17.8816097	17.8832127
800.00	0.0000000	0.0000000	0.0011481	0.0000822	-0.0004549	-0.0000143	-0.0016030	-0.0000896
900.00	18.4428908	18.4427379	14.3485942	14.3478323	33.6596596	33.6605661	19.3110654	19.3127337
1000.00	0.0001529	0.0000083	0.0007619	0.0000531	-0.0009065	-0.0000269	-0.0016684	-0.0000864
1100.00	19.9927981	19.9927417	14.8890429	14.8884219	35.9211153	35.9217548	21.0320524	21.0333330
1200.00	0.0000564	0.0000028	0.0006410	0.0000431	-0.0006396	-0.0000178	-0.0012806	-0.0000609
1300.00	21.5527698	21.5527326	15.4769318	15.4770866	38.1080949	38.1091833	22.6311631	22.6320967
1400.00	0.0000372	0.0000017	-0.0001548	-0.0000100	-0.0010885	-0.0000286	-0.0009336	-0.0000413
1500.00	23.0976450	23.0977521	16.1001885	16.0994725	40.2351917	40.2356566	24.1350032	24.1361841
1600.00	-0.0001071	-0.0000046	0.0007160	0.0000445	-0.0004648	-0.0000116	-0.0011808	-0.0000489
1700.00	23.4649931	23.4649481	16.2481880	16.2474895	40.7202926	40.7205117	24.4721046	24.4730222
1800.00	0.0000450	0.0000019	0.0006985	0.0000430	-0.0002191	-0.0000054	-0.0009176	-0.0000375

MAX REL ERR CP/R = 0.000008 TEMP = 800. AVER REL ERR CP/R = 0.000003 REL LST SQ ERR CP/R = 0.000004
 MAX REL ERR HH/RT = 0.000082 TEMP = 723. AVER REL ERR HH/RT = 0.000046 REL LST SQ ERR HH/RT = 0.000051
 MAX REL ERR S/R = 0.000029 TEMP = 1000. AVER REL ERR S/R = 0.000017 REL LST SQ ERR S/R = 0.000019
 MAX REL ERR GH/RT = 0.000090 TEMP = 723. AVER REL ERR GH/RT = 0.000061 REL LST SQ ERR GH/RT = 0.000064
 MAX ERR CP/R = 0.000153 TEMP = 800. AVER ERR CP/R = 0.000066 LST SQ ERR CP/R = 0.000083
 MAX ERR HH/RT = 0.001148 TEMP = 723. AVER ERR HH/RT = 0.000687 LST SQ ERR HH/RT = 0.000745
 MAX ERR S/R = 0.001088 TEMP = 1000. AVER ERR S/R = 0.000629 LST SQ ERR S/R = 0.000694
 MAX ERR GH/RT = 0.001668 TEMP = 800. AVER ERR GH/RT = 0.001264 LST SQ ERR GH/RT = 0.001298
 CP/R = -1.1212220e+08T**2.0 6.4050666e+05T**1.0 -1.4442432e+03T**0.0 1.6431542e+00T**1.0 -9.0577776e-04T**2.0
 (H-H0)/R CONSTANT = -0.36465252e+07, H/R CONSTANT = -0.37850275e+07, S/R CONSTANT = 0.93420894e+04

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

HA2C03(2) JANAF DATA, MARCH 1966.

1 J 3/66 HA	2.00C	1.000	3.00	0.00	0.00 2	105.98874	-1130767.840
723.150	1123.150	6	-2.0	-1.0	0.0	1.0	2.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
-1.12122199d+08	6.40506661d+05	-1.44424316d+03	1.64315419d+00	-9.05777755d-04			
2.00034993d-07	0.00000000d+00	0.00000000d+00	-3.78502749d+06	9.34208940d+03			

T 1123.15 T 6000. C1 45.30 E1 0.0

TCOEFF

FINISH

COEFFICIENTS ADJUSTED TO FIT UPPER PHASE AT 1123.15

HA2C03(1) HA2C03(2) HA2C03(L)

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

HA2C03(L) JANAF DATA, MARCH 1966.

1 J 3/66 HA	2.00C	1.000	3.00	0.00	0.00 3	105.98874	-1130767.840
1123.150	6000.000	1	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2.27957150d+01	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00	0.00000000d+00
0.00000000d+00	0.00000000d+00	0.00000000d+00	-1.42289169d+05	-1.16217533d+02			

ORIGINAL HA2C03(1) HA2C03(2) HA2C03(L)

ORIGINAL	NA2CO3(1)		NA2CO3(2)		NA2CO3(L)		
T DEG-K	CP J/MOL-K	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K
0	-----	-20.811	-----	-----	-1151.579	-1124.585	-----
100	61.241	-18.192	43.237	225.158	-1148.960	-1129.073	575.9119
200	94.140	-10.142	97.768	148.478	-1140.910	-1130.627	280.8333
298.15	111.002	0.000	138.796	138.796	-1130.768	-1130.768	183.6185
300	111.253	0.205	139.486	138.803	-1130.563	-1130.765	182.3971
* 400	125.102	11.996	173.305	143.317	-1118.772	-1135.691	133.1291
500	142.214	25.338	203.008	152.331	-1105.430	-1134.481	103.4801
600	163.302	40.593	230.760	163.105	-1090.175	-1131.600	83.7484
700	187.569	58.116	257.722	174.699	-1072.652	-1126.656	69.7019
723.15	193.384	62.526	263.918	177.455	-1068.242	-1125.185	67.0121
723.15	143.762	63.216	264.873	177.455	-1067.552	-1124.494	67.0121
800	153.344	74.630	279.864	186.576	-1056.138	-1122.900	59.2148
900	166.230	90.605	298.666	197.995	-1040.163	-1119.841	51.0787
1000	179.201	107.872	316.850	208.978	-1022.896	-1115.648	44.5907
1100	192.046	126.440	334.536	219.590	-1004.327	-1110.316	39.3048
1123.15	195.100	130.922	338.569	222.003	-999.846	-1108.925	38.2188
1123.15	189.535	160.586	364.981	222.003	-970.182	-1079.260	38.2188
1200	189.535	175.152	377.525	231.566	-955.616	-1075.023	35.0107
1400	189.535	213.059	406.742	254.558	-917.709	-1064.586	28.3572
1600	189.535	250.966	432.051	275.198	-879.802	-1055.196	23.4137
1800	189.535	288.873	454.375	293.890	-841.895	-1047.130	19.6006
2000	189.535	326.780	474.345	310.955	-803.988	-1040.691	16.5716
2200	189.535	364.687	492.410	326.643	-766.081	-1036.189	14.1062
2400	189.535	402.594	508.901	341.154	-728.174		
2600	189.535	440.501	524.072	354.649	-690.267		
2800	189.535	478.408	538.118	367.258	-652.360		
3000	189.535	516.315	551.195	379.090	-614.453		
3200	189.535	554.222	563.427	390.233	-576.546		
3400	189.535	592.129	574.918	400.762	-538.639		
3600	189.535	630.036	585.751	410.741	-500.731		
3800	189.535	667.943	595.999	420.224	-462.824		
4000	189.535	705.850	605.721	429.258	-424.917		
4200	189.535	743.757	614.968	437.883	-387.010		
4400	189.535	781.665	623.785	446.134	-349.103		
4600	189.535	819.572	632.211	454.043	-311.196		
4800	189.535	857.479	640.277	461.636	-273.289		
5000	189.535	895.386	648.014	468.937	-235.382		
5200	189.535	933.293	655.448	475.969	-197.475		
5400	189.535	971.200	662.601	482.749	-159.568		
5600	189.535	1009.107	669.494	489.296	-121.661		
5800	189.535	1047.014	676.145	495.625	-83.754		
6000	189.535	1084.921	682.571	501.750	-45.847		

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE,
NA-- 371.010

ORIGINAL	NA2CO3(1)	NA2CO3(2)	NA2CO3(L)
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TABLE I. - FILL PROCEDURE PARAMETERS

Atomic number	Chemical symbol	$\sum_i g_i$	b (or c*)	Atomic number	Chemical symbol	$\sum_i g_i$	b (or c*)
1	H	2	2	38	Sr	670	4
2	He	1	4	39	Y	1260	a ₁₁₇₀
3	Li	8	2	40	Zr	3855	a ₃₇₈₀
4	Be	13	4	41	Nb	7992	a ₈₁₀₀
5	B	6	2	42	Mo	11676	a ₁₂₀₉₆
6	C	15	12	43	Te	12216	a ₁₂₈₅₂
7	N	20	30	44	Ru	9135	a ₉₇₂₀
8	O	15	40	45	Rh	4780	a ₅₁₃₀
9	F	6	30	46	Pd	1666	a ₁₈₀₀
10	Ne	1	12	47	Ag	394	2
11	Na	18	2	48	Cd	125	4
12	Mg	33	4	49	In	92	2
13	Al	16	2	50	Sn	351	12
14	Si	75	12	51	Sb	860	30
15	P	170	30	52	Te	1135	40
16	S	215	40	53	I	846	30
17	Cl	156	30	54	Xe	337	12
18	Ar	61	12	55	Cs	124	2
19	K	42	2	56	Ba	1138	4
20	Ca	426	4	57	La	2200	a ₁₁₇₀
21	Sc	1260	a ₁₁₇₀	Lanthanide series-4f shell filled			
22	Ti	3855	a ₃₇₈₀	72	Hf	3855	a ₃₇₈₀
23	V	7992	a ₈₁₀₀	73	Ta	7992	a ₈₁₀₀
24	Cr	11676	a ₁₂₀₉₆	74	W	11676	a ₁₂₀₉₆
25	Mn	12216	a ₁₂₈₅₂	75	Re	12216	a ₁₂₈₅₂
26	Fe	9135	a ₉₇₂₀	76	Os	9135	a ₉₇₂₀
27	Co	4780	a ₅₁₃₀	77	Ir	4780	a ₅₁₃₀
28	Ni	1666	a ₁₈₀₀	78	Pt	1666	a ₁₈₀₀
29	Cu	362	2	79	Au	434	2
30	Zn	61	4	80	Hg	205	4
31	Ga	30	2	81	Tl	132	2
32	Ge	159	12	82	Pb	591	12
33	As	380	30	83	Bi	1460	30
34	Se	495	40	84	Po	1935	40
35	Br	366	30	85	At	1446	30
36	Kr	145	12	86	Rn	577	12
37	Rb	74	2				

^aThis is the c* value which represents the total quantum weight for each value of n above the ground state principal quantum number. In BLOCK DATA, these values are given as negative values in order for the PAC91 program to differentiate the b values from the c* values.

TABLE 11. - SOME TERMS IN $\ln Q$ AND THEIR DERIVATIVES

For- mula number	Method				Sub- script in equation (9)	ln Q ^m terms	T d(ln Q ^m)/dT terms	T ² d ² (ln Q ^m)/dT ² terms	Remarks		
	RRHO ^a	PANDK ^b and JANAF ^c	NRRAO1 ^d	NRRAO2 ^e					Type of molecule		
									Di- atomic	Linear poly- atomic	Non- linear
1	Yes	Yes	Yes	Yes	e	ln g _m - $\frac{c_2 T_0}{T}$	$\frac{c_2 T_0}{T}$	$-\frac{2c_2 T_0}{T}$	Yes	Yes	C ₂ = hc/k g _m = statistical weight T ₀ = electronic excitation energy
2	Yes	Yes	Yes	Yes	v	$\sum_{i=1}^n d_i \ln(s_i)$	$\sum_{i=1}^n d_i u_i r_i s_i$	$\sum_{i=1}^n d_i u_i r_i s_i (u_i s_i - 2)$	Yes	Yes	d _i = degeneracy n = number of unique frequencies u _i = c ₂ v _i /T r _i = e ^{-u_i} s _i = 1/(1 - r _i) v _i = ω _e - 2ω _x e _e + 3.25ω _y e _e + 5ω _z e _e
3	Yes	Yes	Yes	Yes	R	For diatomic and linear molecules, $\frac{c_2 B_0 \sigma}{T} - \ln \frac{c_2 T_0}{T}$	1	-1	Yes	No	σ = symmetry number B ₀ = B _e - $\frac{\alpha_1}{2} + \frac{\alpha_2}{4} + \frac{\alpha_3}{8}$
4	Yes	Yes	Yes	Yes	R	For nonlinear molecules, $\frac{1}{2} \ln \left[\frac{\pi}{\sigma^2 A_0 B_0 C_0} \left(\frac{T}{c_2} \right)^3 \right]$	3/2	-3/2	No	Yes	A ₀ = A _e - $\frac{1}{2} \sum_{i=1}^n d_i \alpha_i$ B ₀ = B _e - $\frac{1}{2} \sum_{i=1}^n d_i \alpha_i$ C ₀ = C _e - $\frac{1}{2} \sum_{i=1}^n d_i \alpha_i$
5	No	Yes	No	No	p	For JANAF only, ρT	ρT	0	Yes	No	This line for JANAF only; $\rho = 4 \left(\frac{D_0}{g} \right)^{1/2} \frac{v_1 c_2}{D_0}$ ρ is given or $\rho = \frac{D_0}{c_2 B_0^2}$ (except for JANAF)
5a	No	Yes	Yes	Yes	p	For diatomic and linear poly- atomic, $2\rho T + 10\rho^2 T^2 + \frac{296\rho^3 T^3}{3} - \frac{2D_0}{3B_0}$	$2\rho T + 20\rho^2 T^2 + 296\rho^3 T^3$	$20\rho^2 T^2 + 592\rho^3 T^3$	Yes	No	D ₀ = D _e - $\frac{\beta_1}{2} + \frac{\beta_2}{4} + \frac{\beta_3}{8}$; if not given, D _e = $\frac{4B_e^3}{\omega_e^2}$ D ₀ = D ₀₀₀

$c_2 = hc/k$
 g_m = statistical weight
 T_0 = electronic excitation energy

d_i = degeneracy
 n = number of unique frequencies
 $u_i = c_2 \nu_i / T$
 $r_i = e^{-u_i}$
 $s_i = 1/(1 - r_i)$

$\nu_i = \omega_e - 2\omega_e x_e + 3.25\omega_e y_e + 5\omega_e z_e$
 σ = symmetry number
 $B_0 = B_e - \frac{\alpha_1}{2} + \frac{\alpha_2}{4} + \frac{\alpha_3}{8}$

$A_0 = A_e - \frac{1}{2} \sum_{i=1}^n d_i \alpha_i^A$
 $B_0 = B_e - \frac{1}{2} \sum_{i=1}^n d_i \alpha_i^B$
 $C_0 = C_e - \frac{1}{2} \sum_{i=1}^n d_i \alpha_i^C$

This line for JANAF only;
 $\rho = 4 \left(\frac{D_0}{B_0} \right)^{1/2} / \nu_1 c_2$
 ρ is given or $\rho = \frac{D_0}{c_2 B_0^2}$
(except for JANAF)

$D_0 = D_e - \frac{\beta_1}{2} + \frac{\beta_2}{4} + \frac{\beta_3}{8}$; if not
given, $D_0 = \frac{4B_0^3}{\omega_e^2}$
 $D_0 = D_{000}$

TABLE II. - Concluded.

For- mula number	Method		Sub- script in equation (9)	$\ln Q^m$ terms	$T \frac{d(\ln Q^m)}{dT}$ terms	$T^2 \frac{d^2(\ln Q^m)}{dT^2}$ terms	Type of molecule		Remarks
	RRHO ^a	PAND ^b and JANAF ^c					Di- atomic	Non- linear	
7	No	Yes	Yes	Triatomic linear molecules where Fermi resonance occurs $\left(\frac{C_0}{T}\right)^2 \frac{1}{2} r_1^2 s_2^2 (1 - r_1)$	$\ln Q_m \left(S - \frac{r_1 u_1}{1 - r_1} \right)$	$\ln Q_m \left[\frac{2u_1^2 r_1 s_2^2 (1 + r_1 s_2)}{1 - r_1} + 2u_1^2 r_1 s_2 (1 + r_1 s_2) + S^2 - 2S - 2 \right]$	No	Yes	No Fermi resonance constant $u_m = 2C_0 v_2 / T$ $r_m = e^{-u_m}$ $s_m = 1/(1 - r_m)$ $S = (1 + 2r_m s_m) u_m + 2(r_2 u_2 s_2 - 1)$

^aRigid-Rotator Harmonic-Oscillator approximation.
^bModified Pennington and Kobe method.
^cJoint Army Navy Air Force method.
^dNonrigid-Rotator Anharmonic-Oscillator 1.
^eNonrigid-Rotator Anharmonic-Oscillator 2.

*For symmetrical top molecules, (see ref. 8)

$$\rho_1 = \frac{1}{4C_0 B_0^2} \left[(8 + 4m + 3m^2) D_J + (2m + 3m^2) D_{JK} + 3m^2 D_K \right]$$

$$\rho_2 = \frac{3}{32C_0^2 B_0^4} \left[(128 + 64m + 48m^2 + 40m^3 + 35m^4) D_J^2 + 2(16m + 24m^2 + 30m^3 + 35m^4) D_J D_{JK} + 2(8m^2 + 20m^3 + 35m^4) D_{JK} D_K + 35m^4 D_K^2 \right]$$

where $m = B_0/A_0$.

**For asymmetrical top molecules, (see ref. 8)

$$\rho = -\frac{1}{16C_0} \left[3 \left(\frac{\tau_{aaaa}}{A_0^2} + \frac{\tau_{bbbb}}{B_0^2} + \frac{\tau_{cccc}}{C_0^2} \right) + 2 \left(\frac{\tau_{aabb}}{A_0 B_0} + \frac{\tau_{bbcc}}{B_0 C_0} + \frac{\tau_{acac}}{A_0 C_0} \right) + 4 \left(\frac{\tau_{abab}}{A_0 B_0} + \frac{\tau_{bcbc}}{B_0 C_0} + \frac{\tau_{acac}}{A_0 C_0} \right) \right]$$

For planar molecules $\tau_{bcac} = \tau_{acac} = 0$, and also the following relations hold:

$$\tau_{aacc} - \left(\frac{C_0}{A_0} \right)^2 \tau_{aaaa} + \left(\frac{C_0}{B_0} \right)^2 \tau_{aabb} : \tau_{bbcc} - \left(\frac{C_0}{B_0} \right)^2 \tau_{bbbb} + \left(\frac{C_0}{A_0} \right)^2 \tau_{aabb} : \tau_{cccc} - \left(\frac{C_0}{A_0} \right)^2 \tau_{aacc} + \left(\frac{C_0}{B_0} \right)^2 \tau_{bbcc}$$

TABLE III. - TERMS IN $\ln Q^m$

For- mula number	Method			ln Q ^m terms ^e	Type of molecule			Remarks	
	PANDK ^a and JANAF ^b	NRRAO1 ^c	NRRAO2 ^d		Type of molecule			Definitions	
					Dia- tomic	Linear poly- atomic	Non- linear		
8	No	Yes	Yes	$\sum_{i=1}^n d_i a_i r_i s_i \left[1 + \frac{1}{2} a_i s_i + \frac{1}{6} a_i^2 s_i^2 (1 + r_i) \right]$				d_i = degeneracy $r_i = d^{-u_i}$ $u_i = c_2 v_i / T$ $s_i = 1 / (1 - r_i)$ n = number of unique frequencies $v_1 = \omega_e - 2\omega_e x_e + 3.25\omega_e y_e + 5\omega_e z_e$ $a_1 = (\alpha_1 - \alpha_2 - 0.75\alpha_3) / B_0$	
9	Yes	No	No	$\sum_{i=1}^n d_i p_i r_i s_i$	Yes No Yes	No Yes No	No Yes No	$a_i = \frac{B}{B_0} - \sum_{j=1}^n \frac{(1 + \delta_{ij}) \alpha_{ij}}{2B_0}$ $a_i = \frac{1}{2} \left(\frac{\alpha_i^A}{A_0} + \frac{\alpha_i^B}{B_0} + \frac{\alpha_i^C}{C_0} \right)$ $P_i = a_i (a_i + 1)$ For PANDK, $a_1 = (\alpha_1 - 2\alpha_2 - 3.25\alpha_3) / B_0$ and for JANAF, $a_1 = (\alpha_1 - \alpha_2 - 0.75\alpha_3) / B_e$	
10	No	Yes	Yes	$\sum_{i=1}^n \left[d_i a_i r_i s_i^2 (a_i s_i + a_i r_i s_i + 1) + \sum_{j=1}^n d_i d_j a_i r_i s_i s_j \right. \\ \left. + \sum_{j=1}^n d_i d_j a_i a_j (1 + \delta_{ij}) r_i r_j s_i^2 s_j \right]$	Yes No No Yes	No Yes No Yes	No Yes Yes Yes	$P_i = a_i \left(\frac{a_i}{2} + 1 \right) + \frac{1}{4} \left[\left(\frac{\alpha_i^A}{A_0} \right)^2 + \left(\frac{\alpha_i^B}{B_0} \right)^2 + \left(\frac{\alpha_i^C}{C_0} \right)^2 \right]$ $a_{11} = \left(-\alpha_2 - \frac{3}{2} \alpha_3 \right) / B_0$ $a_{ij} = \alpha_{ij} / B_0$ $a_{ij} = 0$ $\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}$	

TABLE III. - Continued.

For- mula number	Method		ln Q^m terms ^e		Remarks		
	PANDK ^a and JANAF ^b	NRRAO1 ^c NRRAO2 ^d			Type of molecule		Definitions
					Dia- tomic	Linear poly- atomic	
11	No	Yes	Yes	$a_{111}r_1^3(1 + 4r_1 + r_1^2)$ (diatomics only)	Yes	No	$a_{111} = -\alpha_3/B_0$
12	No	Yes	Yes	$-\frac{C_2}{T} \sum_{i=1}^n d_i(d_j + \delta_{ij})X_{ij}r_i r_j s_i s_j$	Yes	No	For PANDK, $X_{11} = -\omega_e x_e + 4.5\omega_e y_e + 14.5\omega_e z_e$ and for JANAF, $X_{11} = (-\omega_e x_e + 4.5\omega_e y_e + 14.5\omega_e z_e)v_1/\omega_e$
13	No	Yes	Yes	$-\frac{C_2}{T} \sum_{i=1}^n \sum_{j=1}^n d_i(d_j + \delta_{ij})(d_k + \delta_{jk})Y_{ijk}r_i r_j r_k s_i s_j s_k$	No	Yes	$X_{ii} = x_{ii} + (1.5 d_i + 3)y_{iii} + \sum_{k=1}^n \sum_{k \neq i} \frac{d_k}{2} y_{iik}$
14	Yes	No	No	$-\frac{C_2}{T} \sum_{i=1}^n d_i(d_j + \delta_{ij})(X_{ij} + G_i)r_i r_j s_i s_j$	No	Yes	$X_{ij} = x_{ij} + (d_i + 1)y_{iij} + (d_j + 1)y_{ijj} + \sum_{k=1}^n \sum_{k \neq i} \frac{d_k}{2} y_{ijk}$
15	No	Yes	Yes	$-\frac{24C_2}{T} \omega_e z_e s_1^4$ (diatomics only)	Yes	No	$Y_{111} = \omega_e y_e + 8\omega_e z_e$
16	No	Yes	Yes	$-\frac{C_2}{T} \sum_{i=1}^n 2\delta_i r_i s_i^2(1 - 2a_i r_i s_i)$	No	Yes	$Y_{ijk} = y_{ijk}$
17	No	Yes	Yes	$-\frac{C_2}{T} \sum_{i=1}^n d_i(d_j + \delta_{ij})(1 + \delta_{ij})a_{1ij}x_{ij}r_i r_j s_i s_j$	No	Yes	$G_i = 0$ $G_i = \begin{cases} 0 & \text{if } i \neq j \\ (g_{ii} + B_0)/3 & \text{if } i = j \end{cases}$

TABLE III. - Continued.

Formula number	Method		In Q^m terms ^e		Remarks		
	PANDK ^a and JANAF ^b	NRAO1 ^c	NRAO2 ^d		Type of molecule	Definitions	
					Dia-atomic	Linear poly-atomic	Non-linear
18	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n d_i (d_j + \delta_{ij}) (1 + \delta_{ij})^2 r_i r_j s_i^2 s_j^2$			
19	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \mathcal{Q}_{ijk} X_{ij} X_{jk} r_i r_j r_k s_i^2 s_j^2 s_k^2$	Yes	Yes	Yes
20	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \mathcal{Q}_{ijk} X_{ij} Y_{ijk} r_i r_j r_k s_i^2 s_j^2 s_k^2$	Yes	Yes	Yes
21	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n \sum_{l=1}^n \mathcal{Q}_{ijkl} X_{ij} Y_{ikl} r_i r_j r_k r_l s_i^2 s_j^2 s_k^2 s_l^2$	Yes	Yes	Yes
22	No	No	Yes	$\left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n g_{ii}^2 r_i s_i^4 (1 + 8r_i + r_i^2)$			
23	No	No	Yes	$\left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n 28_{ij} X_{ij} r_i r_j s_i^3 s_j [1 + 7\delta_{ij} + r_i (1 + 5\delta_{ij})]$			
24	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n 4a_i [X_{ii} d_i (d_i + 1)]^2 r_i s_i^5$			
25	No	No	Yes	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{i=1}^n \sum_{j=1}^n \mathcal{Q}_{ij} a_i X_{ij}^2 r_i r_j s_i^3 s_j^2$	Yes	Yes	Yes
							$\mathcal{Q}_{ijk} = (2 - \delta_{jk})(1 + \delta_{ij})(1 + \delta_{ik})d_i(d_j + \delta_{ij})(d_k + \delta_{ik})$ $\mathcal{Q}_{ijk} = 2(1 + \delta_{ij})(1 + \delta_{ik} + \delta_{jk})(d_i + \delta_{ij})d_j(d_k + \delta_{ik} + \delta_{jk})$ $\mathcal{Q}_{ijkl} = 2(1 + \delta_{ij})(1 + \delta_{ik} + \delta_{il} + \delta_{jk})(d_i + \delta_{ij})(d_j + \delta_{ik} + \delta_{il})(d_k + \delta_{jk} + \delta_{il})$ $\mathcal{Q}_{ij} = (1 + \delta_{ij})^2 d_i (d_j + \delta_{ij})$

TABLE III. - Concluded.

For- mula number	Method		$\ln Q^m$ terms ^e	Remarks			
	PAND ^a and JANAF ^b	NRRAO1 ^c		NRRAO2 ^d	Definitions		
					Type of molecule	Non- linear	
			Dia- tomic	Linear poly- atomic			
26	No	No	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{j=1}^N \sum_{k=1}^N \mathcal{Q}_{ijk}^a X_{ik} X_{ij} r_i r_j r_k^3 s_i^3 s_j^3 s_k^3 (1 + r_i)$	Yes	Yes	$\mathcal{Q}_{ijk} = (1 + \delta_{ij})(1 + \delta_{ik})d_i(d_j + \delta_{ij})(d_k + \delta_{ik})$	
27	No	No	$\frac{1}{2} \left(\frac{C_2}{T} \right)^2 \sum_{j=1}^N \sum_{k=1}^N \mathcal{Q}_{ijk}^a X_{ik} X_{ij} r_i r_j r_k^2 s_i^2 s_j^2 s_k^2$	Yes	Yes	$\mathcal{Q}_{ijk} = (1 + \delta_{ij})(1 + \delta_{jk})[2 - \delta_{ik}]d_i(d_j + \delta_{ij})[(1 + \delta_{ik})d_k + \delta_{ik} + \delta_{jk} + \delta_{ij}]$	

^aModified Pennington and Kobe method.^bJoint Army Navy Air Force method.^cNonrigid-Rotator Anharmonic-Oscillator 1.^dNonrigid-Rotator Anharmonic-Oscillator 2.

^eDerivatives: $T[d(\ln Q_C^m)/dT] - \sum_j \ln Q_{C,j} S_j$ and $T^2[d^2(\ln Q_C^m)/dT^2] - \sum_j \ln Q_{C,j} \left[\sum_i m_i u_{hi}^2 r_i s_{hi} (r_{hi} s_{hi} + 1) - 2S_j + S_j^2 - p_j \right]$
 where $\ln Q_C^m = \sum_j \ln Q_{C,j}$ and $\ln Q_{C,j}$ is any term in formulas 8 to 27 which has the formula $\ln Q_{C,j} = (c_2/T)^{p_j} C_j \prod_i r_{hi}^m s_{hi}^m$

where $p_j = 0, 1, \text{ or } 2$; C_j is a constant; n_i and m_i are integer exponents; and h_i is an integer subscript, and where

$$S_j = \sum_i u_{hi} (n_i + m_i r_{hi} s_{hi}) - p_j.$$

TABLE IV. - BRIEF DESCRIPTION OF CONTENTS OF INPUT RECORDS

Record ID	Labels	Numerical value	Comments	Optional?
CTEM	T	T, K	Gives temperature schedule for tables calculated from coefficients if different than original data.	Yes
	I	T increment, K	This may be a single value or the beginning or end of an interval.	Yes
			This must be preceded by a lower and followed by a higher T value.	
data	(See table VII)		All data records following a METHOD record must have the same record ID including the possibility of all blanks. Contents of the remainder of the record may vary with method.	No
DATE	(Any six characters)	(blank)	Label will appear in the least-squares coefficients output.	Yes
FINISH	(blank)	(blank)	Indicates the end of a set of input data for a species.	No
formula	See comments	See comments	Chemical formula of species (columns 1 to 12). For remainder of record, see table V. (The word "formula" does not appear on the record.)	No
LISTEF	(blank)	(blank)	Calls for listing contents of EF data sets stored in I/O unit 13.	Yes
LSTSQS	aEXP	T exponent	q_i values in eq. (11).	Yes
	aNOCONS	(blank)	Fit is to be made with no constraints.	Yes
	aNOCP	(blank)	No heat capacities to be used in least-squares fit.	Yes
	aNOH	(blank)	No enthalpies to be used in least-squares fit.	Yes
	aNOS	(blank)	No entropies to be used in least-squares fit.	Yes
	OLD	(blank)	Use "old" polynomial form for eq. (11) (e.g., $q_i = 0.1, 2, 3, 4$).	Yes
	T	T, K	Temperature at the beginning or end of interval to be fit.	Yes
	TCNST	Constraint T, K	Calls for the data at this temperature to be fitted exactly. Numerical value of T must be the same as some value in the T schedule. Default value is 298.15 K.	Yes
	TPROP	Properties T, K	Used in conjunction with NOH and/or NOS. Specifies temperature at which a value of enthalpy and/or entropy is given to obtain integration constants.	Yes
METHOD	-----	-----	See table VI for details.	No
NAME	-----	-----	Columns 7-24 are reserved for species name and columns 25-80 for comments. Both to be included with coefficients. See table VIII.	Yes
OUTPUT	ATM	(blank)	Calls for pressure to be in units of atmospheres. (Default units are bars.)	Yes
	CAL	(blank)	Calls for the energy units in the tables to be calories.	Yes
	CTAB	(blank)	Calls for tables of functions calculated from coefficients.	Yes
	DMLESS	(blank)	Calls for many-figured tables in dimensionless units.	Yes
	EFTAPE	(blank)	Calls for the H_0^0 value as well as the $\Delta_f H_T^0$ and $-(G_T^0 - H_0^0)/RT$ data to be put on I/O units 11 and 13 for future $\log_{10} K$ and $\Delta_f H_T^0$ calculations.	Yes
	INTERM	(blank)	Calls for intermediate output data.	Yes
	JOULES	(blank)	Calls for the energy units in the tables to be joules.	Yes
	LOGK	(blank)	Calls for rounded tables including columns for $\Delta_f H_T^0$ and $\log_{10} K$.	Yes
	LSQS	(blank)	Calls for least-squared fit of functions.	Yes
	MFIC	(blank)	Calls for tables of many-figured functions.	Yes
REFNCE	Any alphanumeric characters	Any alphanumeric characters	-----	Yes
TEMP	T	Temperature, K	This may be a single value or the beginning or end of an interval.	Yes

^aMay require an integer in column 80. See discussion in section "LSTSQS record."

TABLE V. - CONTENTS OF FORMULA RECORDS

Labels 2, 3, or 4		Numerical value	Comments
HF298	Use only one	An assigned enthalpy, $H_{298.15}^0$	Numerically equal to heat of formation at 298.15 K
ASINDH		An assigned enthalpy, H_T^0	Requires corresponding temperature
DELTAH		Heat of formation from the assigned reference elements ($\Delta_f H_T^0$)	Requires corresponding temperature
T	Use only one	Temperature	Not required with HF298
CAL		(Blank)	Units are cal/mol
KCAL		(Blank)	Units are kcal/mol
JOULES		(Blank)	Units are J/mol
KJOULE		(Blank)	Units are kJ/mol
INVCN		(Blank)	Units are cm ³ /mol
EV		(Blank)	Units are eV/mol

TABLE VI. - CONTENTS OF METHOD RECORDS

Type of species	Method code (any label)	Labels 1,2,3, or 4	Numerical value	Comments
All	COEF		(blank)	Calculate functions from empirical equations.
		DMLSS	(blank)	Coefficients on data records are those of eqs. (11) to (13).
		MELTPT	Melting point	See MELTPT under READIN.
		DELTAH	Heat of transition	Used between two phases of the same species; code is on METHOD record of second phase.
		DELTAS	Entropy of transition	May be used in lieu of a heat of transition (see label DELTAH).
		CAL	(blank)	See READIN below.
		JOULES	(blank)	See READIN below.
		KCAL	(blank)	See READIN below.
		KJOULE	(blank)	See READIN below.
			(blank)	Read in functions directly.
All	READIN	H298HO	$H_{298.15}^0 - H_0^0$	Used in obtaining $H_T^0 - H_0^0$ values when $H_T^0 - H_{298.15}^0$ values are given.
		MELTPT	Melting point	Optional information when a set of input data has both solid and liquid phases.
		CAL	(blank)	Energy units of properties on METHOD and following data records are calories.
		JOULES	(blank)	Energy units of properties on METHOD and following data records are joules.
		KCAL	(blank)	Energy units for enthalpies on METHOD and following data records are kilocalories. Other properties are in calories.
		KJOULE	(blank)	Energy units for enthalpies on METHOD and following data records are kilojoules. Other properties are in joules.

TABLE VI. - Concluded.

Type of species	Method code (any label)	Labels 1,2,3, or 4	Numerical value	Comments
Monatomic gases	ALLN		(blank)	Include all levels given in input.
		GLABEL	(blank)	Labels in data records are $g_m = 2J_m + 1$ (eq. (7)).
		FILL	(blank)	See FILL option under FIXEDN.
Monatomic gases	FIXEDN		Highest principal quantum number to be included in calculations	All energy levels whose principal quantum number is less than or equal to this number will be included.
		GLABEL	(blank)	See GLABEL option under ALLN.
		FILL	(blank)	Missing energy levels will be estimated and included as discussed in the section "Inclusion of predicted levels."
Monatomic gases	TEMPER		(blank)	Cut off all levels above "reduced" ionization potential. (See section "Internal Partition Function for Monatomic Gases.")
		GLABEL	(blank)	See GLABEL option under ALLN.
		FILL	(blank)	See FILL option under FIXEDN.
Diatomic and polyatomic gases	ADD	(blank)	(blank)	No labels for this method.
Diatomic and polyatomic gases	JANAF		(blank)	Calculation method of ref. 6 (see tables II and III).
Diatomic and polyatomic gases	WILH	LINE	(blank)	Wilhoit extrapolation method. LINE required only for linear molecules.
Diatomic and polyatomic gases	NRRA01		(blank)	Calculation method of refs. 30 and 31 (see tables II and III).
Diatomic and polyatomic gases	NRRA02		(blank)	Same as NRRA01 with some higher order corrections (see tables II and III).
Diatomic and polyatomic gases	PANDK		(blank)	Calculation method of ref. 29 (see tables II and III).
Diatomic and polyatomic gases	RRHO		(blank)	Rigid-rotator harmonic-oscillator approximation (see table II).

TABLE VII. - CONTENTS OF DATA RECORDS

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
ADD	(Group name) SYMNO STATWT HRCO SRCO	Quantity of that group Symmetry number Statistical weight H_T^0/R correction S_T^0/R correction	The group names are given in table IX. Each group name is followed by the quantity of that group in the species. Taken to be 1 if omitted. Taken to be 1 if omitted. Any adjustment to H_T^0/R . Any adjustment to S_T^0/R .
READIN	T CP CP/R H-HO H-H2 H-HO/T H-H2/T H-HORT H-H2RT S S/R -G-HO -G-H2 -GH0/T -GH2/T -GHORT -GH2RT	Temperature, K C_p^0 C_p^0/R $H_T^0 - H_0^0$ $H_T^0 - H_{298.15}^0$ $(H_T^0 - H_0^0)/T$ $(H_T^0 - H_{298.15}^0)/T$ $(H_T^0 - H_0^0)/RT$ $(H_T^0 - H_{298.15}^0)/RT$ S_T^0 S_T^0/R $-(C_T^0 - H_0^0)$ $-(C_T^0 - H_{298.15}^0)$ $-(C_T^0 - H_0^0)/T$ $-(C_T^0 - H_{298.15}^0)/T$ $-(C_T^0 - H_0^0)/RT$ $-(C_T^0 - H_{298.15}^0)/RT$	One value on each record. Either one of these values on each record. Any one of these values on each record. Any one of these values on each record.
COEF	See comments T Ei (i = 1, 2, ..., or 8) Ci (i = 1, 2, ..., or 8) CH CH/R CH-HO CHHO/R CS CS/R TCOEF	----- Temperature at beginning or end of temperature range q_i in eq. (11) a_i or $a_i \times R$ in eq. (11) $b_1 \times R$ in eq. (12) b_1 (eq. (12)) $b_1 \times R - H_0^0$ (eq. (12)) $b_1 - H_0^0/R$ (eq. (12)) $b_2 \times R$ (eq. (13)) b_2 (eq. (13)) Temperature at beginning or end of temperature range included with coefficient output	First record may be the same as aforementioned READIN record with C_p^0 or C_p^0/R value omitted. The data will be used in obtaining the integration constants, b_1 and b_2 , in eqs. (12) and (13). Two T labels must precede exponents and coefficients for the temperature range. ----- a_i with DMLESS code in METHOD record. Use one if b_1 has not been set by previous enthalpy value. Use one if b_2 has not been set by previous entropy value. Calls for coefficients to be written on I/O units 6 and 10 in same format as least-squares coefficients. Temperature values should be omitted if they are the same as the T values above.
FIXEDN, ALLN, or TEMPER ^a	IP J_m value	Ionization potential in cm^{-1} e_m/hc in cm^{-1} (eq. (7))	Required only with TEMPER. J_m value (1) Does not have to be right or left-adjusted. (2) May be integer, 0, or decimal number (if decimal, it can have only 5 or 0 to right of decimal point). (3) Must not be left blank (if 0, type in 0).

^aFor FILL option (METHOD record) or FIXEDN, the principal quantum number for the data on each record must be in columns 79 to 80, right-adjusted.

TABLE VII. - Continued.

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
RRHO, PANDK, JANAF, NRRAO1, or NRRAO2 ^b	SYMNO	Symmetry number	Taken to be 1 if omitted.
	STATWT	Statistical weight	Taken to be 1 if omitted.
	T0	T ₀ , cm ⁻¹	Use with excited electronic state.
	B0	B ₀ , cm ⁻¹	B _e , B ₀ , or I _B value must be included for all molecules.
	BE	B _e , cm ⁻¹	See comments for label B0. Use only for linear molecules.
	WE	ω _e , cm ⁻¹	Diatomics only.
	WEXE	ω _e x _e , cm ⁻¹	
	WEYE	ω _e y _e , cm ⁻¹	
	WEZE	ω _e z _e , cm ⁻¹	
	WX4	Anharmonic constant one order higher than ω _e z _e , cm ⁻¹	
	ALPHAE	α _e , cm ⁻¹	Diatomics only. α _e ≡ α ₁
	ALPHAi (i ≤ 3)	α _i	$B_v = B_e - \alpha_1 \left(v + \frac{1}{2}\right) + \alpha_2 \left(v + \frac{1}{2}\right)^2 + \alpha_3 \left(v + \frac{1}{2}\right)^3$
	ALFABi (i ≤ 6)	α _i , cm ⁻¹	Linear polyatomics only.
	Aij (i, j ≤ 6)	α _{ij} , cm ⁻¹	$B_{[v]} = B_e - \sum_{i=1}^{n \leq 6} \left[\alpha_i \left(v_i + \frac{d_i}{2}\right) - \sum_{j \geq 1}^{n \leq 6} \alpha_{ij} \left(v_i + \frac{d_i}{2}\right) \left(v_j + \frac{d_j}{2}\right) \right]$
	ALFAAi (i ≤ 6)	α _i ^A , cm ⁻¹	Nonlinear molecules only. $A_{[v]} = A_e - \sum_{i=1}^{n \leq 6} \alpha_i^A \left(v_i + \frac{d_i}{2}\right)$ where v _i and d _i are the vibrational quantum number and degeneracy respectively for the i th fundamental frequency.
	ALFABi (i ≤ 6)	α _i ^B , cm ⁻¹	Nonlinear molecules only. $B_{[v]} = B_e - \sum_{i=1}^{n \leq 6} \alpha_i^B \left(v_i + \frac{d_i}{2}\right)$
	ALFACi (i ≤ 6)	α _i ^C , cm ⁻¹	Nonlinear molecules only. $C_{[v]} = C_e - \sum_{i=1}^{n \leq 6} \alpha_i^C \left(v_i + \frac{d_i}{2}\right)$
	DE	D _e , cm ⁻¹	Diatomics only.
	BETAi (i ≤ 3)	β _i , cm ⁻¹	Diatomics only, where $D_v = D_e - \beta_1 \left(v + \frac{1}{2}\right) + \beta_2 \left(v + \frac{1}{2}\right)^2 + \beta_3 \left(v + \frac{1}{2}\right)^3$
	Vi(d _i) or Vi (i ≤ 20)	v _i (d _i) or v _i , cm ⁻¹	d _i is degeneracy (an integer) of v _i and may be omitted when d _i = 1.
	Xij (i ≤ 6, j ≤ 6)	x _{ij} , cm ⁻¹	Polyatomics only.
	Yijk (i ≤ 6, j ≤ 6, k ≤ 6)	y _{ijk} , cm ⁻¹	Polyatomics only.
	W0	W ₀ (Fermi resonance constant), cm ⁻¹	Linear polyatomics only.
	Gii (i ≥ 6)	g _{ii} , cm ⁻¹	Linear polyatomics only.
	D0 or D000	D ₀ or D ₀₀₀	Polyatomics only.
	RHO	ρ, K ⁻¹	Polyatomics only.
	A0	A ₀ , cm ⁻¹	An I _A or A ₀ must be included for all nonlinear polyatomics.
	C0	C ₀ , cm ⁻¹	An I _C or C ₀ must be included for all nonlinear polyatomics.
	IB	I _B × 10 ³⁹ , (g)(cm ²)	B ₀ = h/8π ² cI _B = 2.7992774 × 10 ⁻³⁹ /I _B . See comments for label B0.
	IA	I _A × 10 ³⁹ , (g)(cm ²)	A ₀ = h/8π ² cI _A = 2.7992774 × 10 ⁻³⁹ /I _A . See comments for label A0.
	IC	I _C × 10 ³⁹ , (g)(cm ²)	C ₀ = h/8π ² cI _C = 2.7992774 × 10 ⁻³⁹ /I _C . See comments for label C0.

^bFor excited electronic states, the data for each state should be put on separate records with an identifying number in columns 79 to 80. Data records for each state must be grouped together.

TABLE VII. - Concluded.

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
RRHO, PANDK, JANAF, NRRAO1, or NRRAO2 ^b (concluded)	IAIBIC	$I_A I_B I_C \times 10^{117}, (g)^3 (cm)^6$	Replaces individual values for I_A , I_B , and I_C .
	INTROT	Total number of internal rotors	Remaining labels in this table, which appear on records following the INTROT record, are parameters pertaining to internal rotation. Integer in column 79 or 80 indicates to which rotor parameters belong (maximum of four unique rotors).
	ANGLES	<201	The number of phase angles in 2π radians (see eq. (10)). If number is not assigned, default value is 201.
	BROT	B_0, cm^{-1}	Same as B_0 but for internal rotation $BROT = 2.7992774 \times 10^{-39} / I_B$.
	NEL	<187	Number of energy levels to be calculated. Default is 187.
	NOUT	<187	Number of energy levels to be printed. Default is 0.
	NROTOR	1, 2, 3, or 4	Integer specifying the number of rotors with identical parameters.
	ROSYM	Rotor symmetry number	
	V	Potential, cm^{-1}	See eq. (10).
	V_n ($n \leq 6$)	V_n	n-fold barrier V_n (see eq. (10)).
	IPRINT		Calls for listing the potential corresponding to the various phase angles. (Not used to obtain the partition function.)

^bFor excited electronic states, the data for each state should be put on separate records with an identifying number in columns 79 to 80. Data records for each state must be grouped together.

TABLE VIII. - GENERAL THERMODYNAMIC COEFFICIENTS FORMAT

General Format:

Record	Contents	Format	Columns
1	Species name or formula Comments - data source	A24 A56	1 to 24 25 to 80
2	Number of T intervals Optional identification code Chemical formula, symbols and numbers 0 for gas and non-zero for condensed Molecular weight Heat of formation at 298.15 K, J/mol	I2 A6 5(A2,F6.2) I1 F13.5 F15.3	2 4 to 9 11 to 50 52 53 to 65 66 to 80
3	Temperature range Number of coefficients for C_p^o T exponents in empirical equation for C_p^o $H_{298.15}^o - H_0^o$, J/mol	2F10.3 I1 8F5.1 F15.3	2 to 21 23 24 to 63 66 to 80
4	First five coefficients	5D16.8	1 to 80
5	Last three coefficients for C_p^o Integration constants for H_T^o/RT and S_T^o/R	3D16.8 2D16.8	1 to 48 49 to 80
...	Repeat 3, 4, and 5 for each interval.		

Example:

SIH+ SILYLIDYNE ION. JANAF DEC, 1971.

```

2 J12/71 SI  1.00H  1.00E -1.00   0.00   0.00 0   29.09289   1147671.200
  298.150 1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0   8654.259
-4.28447370d+04  3.85838948d+02  2.55865994d+00 -6.98804091d-04  5.22573029d-06
-4.84510719d-09  1.45288897d-12  0.00000000d+00  1.34921190d+05  8.95659370d+00
 1000.000 6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0   8654.259
 1.70438606d+05 -1.04392569d+03  4.83677344d+00  1.28725833d-04 -6.90835693d-08
 1.42207295d-11 -7.87210915d-16  0.00000000d+00  1.43159900d+05 -7.53965976d+00

```

Empirical equations for above example (from eqs. (11) to (13)):

$$\text{Heat capacity: } \frac{C_p^o}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4$$

$$\text{Enthalpy: } \frac{H_T^o}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln T + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{b_1}{T}$$

$$\text{Entropy: } \frac{S_T^o}{R} = -a_1 \frac{T^{-2}}{2} - a_2 T^{-1} + a_3 \ln T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + b_2$$

TABLE IX. - GROUP NOTATION AND STRUCTURE

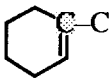
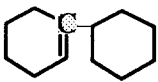
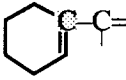
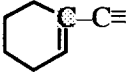
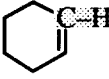
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
1	CA	C _a	$\text{C}=\text{C}=\text{C}$	C	36
2	CBC	C _B - (C)		C	36
3	CBCB	C _B - (C _B)		C	37
4	CBCD	C _B - (C _d)		C	37
5	CBCT	C _B - (C _t)		C	37
6	CBH	C _B - (H)		CH	37
7	CDC2	C _d - (C) ₂	$\text{C}-\overset{\#}{\text{C}}-\text{C}$	C	36
8	CDCBC	C _d - (C _B)(C)	$\text{C}-\overset{\#}{\text{C}}-\text{C}_6\text{H}_9$	C	36
9	CDCDC	C _d - (C _d)(C)	$\text{C}-\overset{\#}{\text{C}}-\text{C}=\text{C}$	C	36
10	CDHC	C _d - (H)(C)	$\text{H}-\overset{\#}{\text{C}}-\text{C}$	CH	36
11	CDHCB	C _d - (C _B)(H)	$\text{H}-\overset{\#}{\text{C}}-\text{C}_6\text{H}_9$	CH	37

TABLE IX. - Continued.




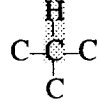
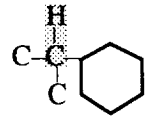
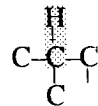
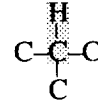
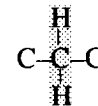
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
12	CDHCD	$C_d - (C_d)(H)$		CH	37
13	CDHCT	$C_d - (C_t)(H)$		CH	37
14	CDH2	$C_d - (H)_2$		CH ₂	37
15	CHC3	$C - (H)(C)_3$		CH	36
16	CHCBC2	$C - (C_B)(C)_2(H)$		CH	36
17	CHCDC2	$C - (C_d)(C)_2(H)$		CH	36
18	CHCTC2	$C - (C_t)(C)_2(H)$		CH	36
19	CH2C2	$C - (H)_2(C)_2$		CH ₂	36

TABLE IX. - Continued.

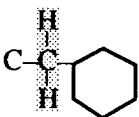
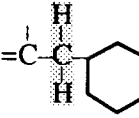
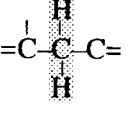
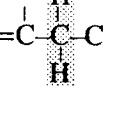


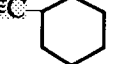
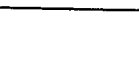
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
20	CH2CBC	$C - (C_B)(C)(H)_2$		CH ₂	36
21	CH2CBD	$C - (C_d)(C_B)(H)_2$		CH ₂	36
22	CH2CD2	$C - (C_d)_2(H)_2$		CH ₂	36
23	CH2CDC	$C - (C_d)(C)(H)_2$		CH ₂	36
24	CH2CTC	$C - (C_t)(C)(H)_2$		CH ₂	36
25	CH3C	$C - (H)_3(C)$		CH ₃	36
26	CTC	$C_t - (C)$		C	36
27	CTCB	$C_t - (C_B)$		C	37

TABLE IX. - Concluded.

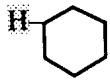
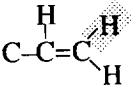
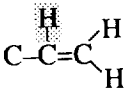
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
28	CTCD	$C_t - (C_d)$	$\equiv C - \overset{ }{C} =$	C	37
29	CTCT	$C_t - (C_t)$	$\equiv C - C \equiv$	C	37
30	CTH	$C_t - (H)$	$\equiv C - H$	CH	37
31	HC2H	H - ACETYL	$H - C \equiv C - H$	H	see "Input"
32	HPHEN	H - PHENYL		H	see "Input"
33	HVIN	H - VINYL		H	see "Input"
34	HVINS	H - STABILIZED VINYL		H	see "Input"

TABLE X. - GROUP ADDITIVITY COEFFICIENTS

CA

2 BEN76 C	1.00	0.00	0.00	0.00	0.00	0	12.01100	17210.010
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
6.20131064d-01	6.55685438d-03	-8.40971939d-06	5.34237173d-09	-1.34221334d-12	1.67980617d+04	-2.13964424d+00		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
1.70014134d+00	2.13036557d-03	-1.46491180d-06	4.57867726d-10	-5.30959813d-14	1.65796625d+04	-7.34011722d+00		

CBC

2 BEN76 C	1.00	0.00	0.00	0.00	0.00	0	12.01100	2772.724
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
1.10379898d+00	-1.40207754d-03	1.01721889d-05	-1.04915786d-08	3.35530569d-12	2.43522265d+03	-1.01067689d+01		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
1.18859776d+00	2.62679100d-03	-1.40397450d-06	3.62315999d-10	-3.62315999d-14	2.15954456d+03	-1.17034055d+01		

CBCB

2 S&F85 C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
-9.07225320d-01	1.21274570d-02	-1.59921140d-05	1.06772290d-08	-2.88771260d-12	2.34891290d+03	-2.17231890d+00		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
1.64937250d+00	2.43505820d-03	-1.40110120d-06	3.74624350d-10	-3.82283850d-14	1.78059830d+03	-1.47139470d+01		

CBCD

2 S&F85 C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
1.89361290d+00	-3.63320180d-03	1.33476670d-05	-1.32062840d-08	4.38875210d-12	2.36121080d+03	-1.41160640d+01		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
6.57951850d-01	3.79153180d-03	-2.18052300d-06	5.80353650d-10	-5.87829120d-14	2.50341600d+03	-8.72472110d+00		

CBCT

2 S&F85 C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
1.89361290d+00	-3.63320180d-03	1.33476670d-05	-1.32062840d-08	4.38875210d-12	2.36121080d+03	-1.58018030d+01		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
6.57951850d-01	3.79153180d-03	-2.18052300d-06	5.80353650d-10	-5.87829120d-14	2.50341600d+03	-1.04104590d+01		

CBH

2 S&F85 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
-8.59079180d-01	1.01575080d-02	-6.05790130d-06	1.11817290d-10	8.76799660d-13	1.51812920d+03	7.93471810d+00		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
8.12920500d-01	5.70326930d-03	-2.94688640d-06	7.32625720d-10	-7.11722860d-14	1.07063610d+03	-6.86258470d-01		

CDC2

2 BEN76 C	1.00	0.00	0.00	0.00	0.00	0	12.01100	5203.260
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
1.57567141d-02	1.20990725d-02	-2.39398157d-05	2.39017773d-08	-9.01711547d-12	4.82932602d+03	-9.21726687d+00		
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
2.25642353d+00	1.36203978d-03	-7.27986777d-07	1.87867555d-10	-1.87867555d-14	4.34871092d+03	-1.99090723d+01		

TABLE X. - Continued.

CDCBC									
2 BEN76 C	1.00	0.00	0.00	0.00	0.00	0	12.01100	4347.792	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
-2.15050677d+00	2.56218701d-02	-4.82075840d-05	4.17875044d-08	-1.37198166d-11					
			4.19996194d+03	-9.32804085d-01					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
3.04446083d+00	4.86442777d-04	-2.59995277d-07	6.70955554d-11	-6.70955554d-15					
			3.27765919d+03	-2.51782099d+01					
CDCDC									
2 BEN76 C	1.00	0.00	0.00	0.00	0.00	0	12.01100	4468.564	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
-2.15050677d+00	2.56218701d-02	-4.82075840d-05	4.17875044d-08	-1.37198166d-11					
			4.32073394d+03	-9.32804085d-01					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
3.04446083d+00	4.86442777d-04	-2.59995277d-07	6.70955554d-11	-6.70955554d-15					
			3.39843119d+03	-2.51782099d+01					
CDHC									
2 BEN76 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	4322.631	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
3.87658435d-01	6.91462635d-03	-4.92473068d-06	3.06564147d-09	-1.19103098d-12					
			3.93773106d+03	-6.55229555d-02					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
1.76953318d+00	3.63735034d-03	-1.32392850d-06	1.71399542d-10	-2.18997389d-15					
			3.48001920d+03	-7.46676354d+00					
CDHCB									
2 S&F85 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	0.000	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
-1.77479380d+00	2.03672900d-02	-2.92063140d-05	2.13900470d-08	-6.19476560d-12					
			3.25431500d+03	8.37139370d+00					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
2.16078460d+00	3.89973620d-03	-1.87505280d-06	4.40575310d-10	-4.10819930d-14					
			2.44872450d+03	-1.05679580d+01					
CDHCD									
2 S&F85 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	0.000	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
-1.77479380d+00	2.03672900d-02	-2.92063140d-05	2.13900470d-08	-6.19476560d-12					
			3.25431500d+03	8.37139370d+00					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
2.16078460d+00	3.89973620d-03	-1.87505280d-06	4.40575310d-10	-4.10819930d-14					
			2.44872440d+03	-1.05679580d+01					
CDHCT									
2 S&F85 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	0.000	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
-1.77479380d+00	2.03672900d-02	-2.92063140d-05	2.13900470d-08	-6.19476560d-12					
			3.25431500d+03	9.20168260d+00					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
2.16078460d+00	3.89973620d-03	-1.87505280d-06	4.40575310d-10	-4.10819930d-14					
			2.44872450d+03	-9.73766950d+00					
CDH2									
2 S&F85 C	1.00H	2.00	0.00	0.00	0.00	0	14.02688	0.000	
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0		
7.08636360d-01	5.71738370d-03	3.97432860d-06	-8.14882140d-09	3.39759220d-12					
			2.66405290d+03	8.03997270d+00					
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0		
7.62035270d-01	7.90072810d-03	-3.83366760d-06	9.04921890d-10	-8.42780610d-14					
			2.55458540d+03	7.24431290d+00					

TABLE X. - Continued.

CHC3

2 BEN76 C 1.00H 1.00 0.00 0.00 0.00 0 13.01894 -956.112
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -1.21199942d+00 1.57135839d-02 -1.58129928d-05 8.16308832d-09 -1.79427286d-12
 -1.16875169d+03 -3.21908314d+00
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 4.21180248d+00 8.18242540d-05 1.33950798d-06 -6.69862359d-10 9.41347774d-14
 -2.66361789d+03 -3.11576551d+01

CHCBC2

2 BEN76 C 1.00H 1.00 0.00 0.00 0.00 0 13.01894 -493.152
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -2.70626696d+00 2.55442809d-02 -3.35585641d-05 2.09055818d-08 -5.02705367d-12
 -5.64094599d+02 3.00591586d+00
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 3.92458678d+00 2.09170394d-03 -1.11797969d-06 2.88510888d-10 -2.88510888d-14
 -2.12756082d+03 -2.99433080d+01

CHCDC2

2 BEN76 C 1.00H 1.00 0.00 0.00 0.00 0 13.01894 -744.761
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -2.69178809d+00 2.27174202d-02 -2.67597650d-05 1.50516772d-08 -3.18914467d-12
 -7.43740880d+02 3.74363064d+00
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 2.00129268d+00 5.30222627d-03 -2.83394852d-06 7.31341554d-10 -7.31341554d-14
 -1.74761503d+03 -1.92282945d+01

CHCTC2

2 BEN76 C 1.00H 1.00 0.00 0.00 0.00 0 13.01894 -865.533
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -2.29967144d+00 2.07315703d-02 -2.60278088d-05 1.75696487d-08 -4.99182528d-12
 -9.03749304d+02 2.30198068d+00
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 1 1.48247630d+00 5.93460188d-03 -3.17194238d-06 8.18565776d-10 -8.18565777d-14
 -1.70025797d+03 -1.60989330d+01

CH2C2

2 BEN76 C 1.00H 2.00 0.00 0.00 0.00 0 14.02688 -2480.858
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 2.95576901d-01 8.26548665d-03 2.02730929d-06 -8.22251499d-09 3.84394234d-12
 -2.93983603d+03 5.66809199d-01
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 8.95359335d-01 8.82630650d-03 -4.51610338d-06 1.11218836d-09 -1.07950628d-13
 -3.18218807d+03 -2.98904913d+00

CH2CBC

2 BEN76 C 1.00H 2.00 0.00 0.00 0.00 0 14.02688 -2445.633
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -1.61079486d+00 2.13020824d-02 -2.44229173d-05 1.42423100d-08 -3.20026830d-12
 -2.72304502d+03 8.49250374d+00
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 2.81096829d+00 5.93460188d-03 -3.17194238d-06 8.18565777d-10 -8.18565777d-14
 -3.81247249d+03 -1.36149824d+01

CH2CBD

2 BEN76 C 1.00H 2.00 0.00 0.00 0.00 0 14.02688 -2158.799
 298.150 1000.000 5 0.0 1.0 2.0 3.0 4.0
 -2.99489148d+00 2.49586869d-02 -2.77613624d-05 1.47398773d-08 -2.60172081d-12
 -2.15783856d+03 1.58638825d+01
 1000.000 3000.000 5 0.0 1.0 2.0 3.0 4.0
 1.17752700d+00 8.75596999d-03 -4.67991499d-06 1.20772000d-09 -1.20772000d-13
 -3.03586486d+03 -4.40568818d+00

TABLE X. - Continued.

CH2CD2										
2	BEN76	C	1.00H	2.00	0.00	0.00	0.00	0	14.02688	-2158.799
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
-2.99489148d+00	2.49586869d-02	-2.77613624d-05	1.47398773d-08	-2.60172081d-12						
			-2.15783856d+03	1.58638825d+01						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
1.17752700d+00	8.75596999d-03	-4.67991499d-06	1.20772000d-09	-1.20772000d-13						
			-3.03586486d+03	-4.40568818d+00						
CH2CDC										
2	BEN76	C	1.00H	2.00	0.00	0.00	0.00	0	14.02688	-2395.311
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
-9.84166104d-01	1.41467063d-02	-7.15413971d-06	-2.15080256d-09	2.42261065d-12						
			-2.66434595d+03	6.65325780d+00						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
8.87674198d-01	9.14512421d-03	-4.88791121d-06	1.26139644d-09	-1.26139644d-13						
			-3.13410437d+03	-2.90870113d+00						
CH2CTC										
2	BEN76	C	1.00H	2.00	0.00	0.00	0.00	0	14.02688	-2380.215
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
-7.61851269d-01	1.30343429d-02	-7.51763250d-06	4.44629802d-10	9.34733367d-13						
			-2.66730666d+03	5.96602298d+00						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
3.68857816d-01	9.77749982d-03	-5.22590507d-06	1.34862066d-09	-1.34862066d-13						
			-2.94558197d+03	2.32409280d-01						
CH3C										
2	BEN76	C	1.00H	3.00	0.00	0.00	0.00	0	15.03482	-5132.810
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
9.67091211d-01	4.54272496d-03	1.40931220d-05	-2.03529587d-08	8.18255263d-12						
			-5.71121159d+03	7.97556073d+00						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
-6.27511183d-01	1.36690420d-02	-7.30586729d-06	1.88538511d-09	-1.88538511d-13						
			-5.43213903d+03	1.52438529d+01						
CTC										
2	BEN76	C	1.00	0.00	0.00	0.00	0.00	0	12.01100	13863.619
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
8.02437417d-01	3.49837285d-03	-4.15397270d-06	4.07988802d-09	-1.75083632d-12						
			1.34983448d+04	-2.26753348d+00						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
1.24244195d+00	2.09170394d-03	-1.11797969d-06	2.88510888d-10	-2.88510888d-14						
			1.33531243d+04	-4.58500863d+00						
CTCB										
2	S&F85	C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
-3.49384520d+00	2.72321320d-02	-4.76891040d-05	3.86559630d-08	-1.19225380d-11						
			1.33155360d+04	1.68245410d+01						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
2.28560130d+00	8.22574900d-04	-4.14361390d-07	1.03588260d-10	-1.03983680d-14						
			1.22382860d+04	-1.04535180d+01						
CTCD										
2	S&F85	C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0			
7.72587840d-01	1.44159610d-03	2.24535910d-06	-3.27337130d-09	1.18176800d-12						
			1.38820450d+04	-1.66930970d+00						
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0			
4.49136330d-01	3.36057940d-03	-1.88820530d-06	4.95862840d-10	-4.98295890d-14						
			1.39278700d+04	-2.35699140d-01						

TABLE X. - Concluded.

CTCT

2 S&F85 C	1.00H	0.00	0.00	0.00	0.00	0	12.01100	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
9.09050340d-03	9.68282400d-03		-1.61930660d-05	1.34477210d-08	-4.31250880d-12			
				1.25675030d+04	6.29563560d-01			
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
1.61375010d+00	1.75286410d-03		-9.50741270d-07	2.44108940d-10	-2.42282270d-14			
				1.22902950d+04	-6.81710090d+00			

CTH

2 S&F85 C	1.00H	1.00	0.00	0.00	0.00	0	13.01894	0.000
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	
3.22062990d-01	1.23444940d-02		-1.94881630d-05	1.58382730d-08	-4.95581450d-12			
				1.30498420d+04	7.64972930d+00			
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	
2.08408360d+00	3.00946820d-03		-1.27530500d-06	2.64569910d-10	-2.18420530d-14			
				1.27910130d+04	-3.35539540d-01			

HVIN

C2H4 - C2H3

2 L 2/91 H	1.00	0.00	0.00	0.00	0.00	0	1.00794	-625071.953
200.000	1000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
7.46735360d-01	-9.08531026d-03		3.11780593d-05	-3.33930685d-08	1.22733472d-11			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-7.52125326d+04	-2.33376993d+00			
1000.000	6000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
-3.59257940d-01	2.99014152d-03		-1.07409461d-06	1.73348003d-10	-1.03738147d-14			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-7.53284072d+04	1.23891111d+00			

HVINS

C2H4 - C2H3 + 8 kcal correction on H.

2 L 2/91 H	1.00	0.00	0.00	0.00	0.00	0	1.00794	-591599.953
200.000	1000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
7.46735360d-01	-9.08531026d-03		3.11780593d-05	-3.33930685d-08	1.22733472d-11			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-7.11867993d+04	-2.33376993d+00			
1000.000	6000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
-3.59257940d-01	2.99014152d-03		-1.07409461d-06	1.73348003d-10	-1.03738147d-14			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-7.13026738d+04	1.23891111d+00			

HPHEN

C6H6 - C6H5

2 L 1/91 H	1.00	0.00	0.00	0.00	0.00	0	1.00794	-254320.000
200.000	1000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
-2.06302352d-01	-8.15243200d-04		1.43769315d-05	-1.95955059d-08	8.17474280d-12			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-3.05819013d+04	1.10333770d+00			
1000.000	6000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
3.06920100d-01	2.32195120d-03		-8.16396860d-07	1.29838420d-10	-7.68981960d-15			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-3.08941277d+04	-2.51191430d+00			

HC2H

C2H2 - C2H1

2 L 3/91 H	1.00	0.00	0.00	0.00	0.00	0	1.00794	-331613.472
298.150	1000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
-3.22796852d+00	1.87214852d-02		-3.02272137d-05	2.39352994d-08	-7.26880375d-12			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-3.95302119d+04	1.38493147d+01			
1000.000	3000.000	5	0.0	1.0	2.0	3.0	4.0	0.0 0.0 0.0
-5.51834000d-02	3.11952519d-03		-1.41953706d-06	3.15909714d-10	-2.79158072d-14			
0.00000000d+00	0.00000000d+00		0.00000000d+00	-4.00479060d+04	-8.06478801d-01			

TABLE XI. - INDEX OF INPUT RECORD ID'S AND LABELS

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
ADD	Label	2	VI	6,10,17,18,19,23,24
ALLN	Label		VI,VII	6,10,15,16,19,22
ALPHA _E	Label		VII	
ALPHA _i	Label	7	VII	
ALFA _B _i	Label		VII	
ALFA _i _j	Label		VII	
ALFAA _i	Label	5	VII	
ALFA _B _i	Label	5	VII	
ALFA _C _i	Label	5	VII	
ANGLES ^a	Label		VII	
ASINDH ^a	Label	5	V	18
ATM	Label	3	IV	11,19
AO	Label	5	VII	
BAR	Label	3		11
BE	Label	7	VII	
BETA _i	Label		VII	
BROT	Label		VII	
BO	Label	5	VII	
C _i	Label	6,8	VII	
CAL	Label	1,4,5,8	IV,V,VI	9,19,21
CH	Label		VII	
CH/R	Label		VII	
CH-HO	Label		VII	
CHHO/R	Label		VII	
COEF	Label	6,8	VI,VII	10,11,16,19,24
CP	Label	3,6,8	VII	
CP/R	Label		VII	
CS	Label		VII	
CS/R	Label		VII	
CTAB	Label	1,6,7	IV	9,19,21
CTEM	Record ID	6,7	IV	8,9,12,15,16,21,24
CO	Label	5	VII	

^aProgram checks first four characters only.

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
data	Any record ID	1-8	IV, VI, VII	9, 10, 11, 15, 16, 17, 18, 19, 21
DATE	Record ID	1-4, 6-8	IV	9, 15, 17, 24
DE	Label		VII	
DELTAH	Label	6, 8	V, VI	7, 12, 16
DELTAS	Label		VI	7, 12, 16
DMLESS ^a	Label	1, 3, 4	IV, VI	9, 19, 21
DO	Label		VII	
D000	Label		VII	
Ei	Label	6, 8	VII	
EFDA	Record ID			8, 10, 11, 15, 17, 23
EFTAPE ^a	Label	6	IV	9, 10, 17, 19, 21, 23
EV	Label		V	
EXP	Label	1, 2	IV	7, 10, 18
FILL	Label	1	I, VI, VII	6, 12, 16, 22
FINISH ^a	Record ID	1-8	IV	8, 9, 10, 15, 17, 24
FIXEDN ^a	Label		VI, VII	6, 10, 15, 16, 19, 22
formula ^b	Variable record ID and label	1-8	IV, V	9, 15, 17, 24
-G-HO	Label		VII	
-GH0/T	Label		VII	
-GHORT	Label		VII	
-G-H2	Label		VII	
-GH2/T	Label		VII	
-GH2RT	Label		VII	
Gii	Label		VII	
GLABEL ^a	Label		VI	16
H-HO	Label	3, 6	VII	
H-HO/T	Label		VII	
H-HORT	Label		VII	
H-H2	Label	6, 8	VII	
H-H2/T	Label		VII	

^aprogram checks first four characters only.

^bFirst 12 columns of record are reserved for chemical formula.

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
H-H2RT	Label		VII	
H298H0	Label	2,6,8	VI	16
HF298	Label	1,3,4,6,7,8	V	10,18
HRCO	Label		VII	11,17
I	Label	1,2,4-8	IV	16,20
IA	Label		VII	
IAIBIC ^a	Label	4	VII	
IB	Label	4	VII	
IC	Label		VII	
INTERM ^a	Label	5	IV	10,11,19,22
INVCMA	Label		V	
INTROTA	Label	4	VII	11
IP	Label	1	VII	
IPRINT ^a	Label		VII	
J _m ^c	Numerical label	1	VII	10
JANAF ^a	Label	7	II,III,VI,VII	6,11,16,17,19,22,24
JOULES ^a	Label	1-8	IV,V,VI	9,19,21
KCAL	Label	8	V,VI	
KJOULE ^a	Label	3	V,VI	
LINE	Label		VI	7,19,33
LISTEF ^a	Record ID		IV	8,10,16,18,21,23
LOGK	Label	7,8	IV	9,11,17,18,19,21,23
LSQS	Label	1,2,6,7,8	IV	9,10,11,18,19,21,23
LSTSQS ^a	Record ID	1,2	IV	6,7,8,9,15,16,18,19,40,45
MELTPT ^a	Label	6,8	VI	
METHOD ^a	Record ID	1-8	IV,VI	6,7,8,9,10,11,12,15,16,18,19,20,22,23,24
MFIG	Label	1-6	IV	9,12,19,21
NAME	Record ID	1-4,6-8	IV	8,9,11,15,19,24,30
NEL	Label	4	VII	
NOCNS ^a	Label		IV	7,18

^aProgram checks first four characters only.

^cLabels are numerical values of J_m or g_m (eq. (7)).

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
NOCP	Label		IV	16, 18, 19
NOH	Label		IV	16, 18, 19
NOS	Label		IV	16, 18, 19
NOUT	Label		VII	11
NROTOR ^a	Label	4	VII	
NRRA01	Label		II, III, VI, VII	6, 11, 16, 19, 22, 38
NRRA02	Label	5	II, III, VI, VII	6, 11, 16, 17, 19, 22, 24
OLD	Label		IV	18
OUTPUT ^a	Record ID	1-8	IV	8, 9, 10, 11, 12, 15, 17, 18, 19, 21, 22, 23, 24
PANDK ^a	Label		II, III, VI, VII	6, 8, 11, 16, 19, 22
READIN ^a	Label	3, 6, 8	VI	9, 11, 16, 19, 20, 24
REFNCE ^a	Record ID	1, 3-6	IV	8, 9, 15, 20, 24
RHO	Label	5	VII	
ROSYM ^a	Label	4	VII	
RRHO	Label	4	II, VI, VII	6, 11, 15, 16, 17, 19, 22, 24
S	Label	3, 6, 8	VII	
S/R	Label		VII	
SRCO	Label		VII	
STATWT ^a	Label	2, 4, 5, 7	VII	15
SYMNO ^a	Label	2, 5	VII	
T	Label	1-8	IV, V, VII	10, 16, 18, 19, 20
TCOEF ^a	Label	6, 8	VII	10, 16
TCONST ^a	Label		IV	18
TEMP	Record ID	1-6, 8	IV	8, 9, 12, 15, 16, 19, 20, 24, 45
TEMPER ^a	Label	1	VI, VII	6, 10, 15, 16, 19, 24
TPROP ^a	Label		IV	18
TO	Label	7	VII	
V	Label		VII	
Vi	Label	4, 5	VII	
VN	Label		VII	
WE	Label	7	VII	
WEXE	Label	7	VII	

^aProgram checks first four characters only.

TABLE XI. - Concluded.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
WEYE	Label		VII	7,12,16,19,24
WEZE	Label		VII	
WX4	Label		VII	
WILH	Label	2,3	VI	
WO	Label		VII	
X _{ij}	Label	5	VII	
Y _{ijk}	Label	5	VII	

a_1	a_2	a_3	a_4	a_5	a_6	a_7	$a_8 = \frac{H_0}{T_0}$	b_0	b_1	b_2	Constants
$\sum_{i=1}^n T_i^{-4}$	$\sum (\frac{5}{2} - \ln T) T^{-3}$	$-\frac{1}{2} \sum T^{-2} \ln T$	0	$\frac{5}{12} T$	$\frac{1}{2} \sum T$	$-\frac{1}{2} \sum T^{-2}$	$-\sum T^{-1}$	$\frac{5}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$\sum (\frac{5}{2} - \ln T) T^{-3}$	$\sum [(\frac{5}{2} - \ln T) T^{-2}] T^{-2}$	$\sum T^{-1}$	$\frac{1}{2} \sum \ln T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^2$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^{-1}$	$\sum T^{-1}$	$\frac{5}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$-\frac{1}{2} \sum T^{-2} \ln T$	$\sum T^{-1}$	$\sum [(\frac{5}{2} - \ln T) T^{-2}]$	$\sum (\frac{5}{2} + \ln T) T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^2$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^{-1}$	$\sum T^{-1}$	$\sum T^{-1}$	1	1	$\ln T_0$	$\sum (\frac{5}{2} - \ln T) T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$\frac{1}{12} \sum T$	$\frac{1}{2} \sum \ln T$	$\sum (\frac{5}{2} + \ln T) T$	$\sum T^2$	$\frac{1}{2} \sum T^3$	$\frac{1}{2} \sum T^4$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$\frac{5}{12} T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^2$	$\frac{1}{2} \sum T^3$	$\frac{1}{2} \sum T^4$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} \sum T^{-3}$	$\frac{1}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$\frac{1}{12} \sum T$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^2$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^3$	$\frac{1}{2} \sum T^4$	$\frac{1}{2} \sum T^5$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} \sum T^{-3}$	$\frac{1}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$\frac{23}{48} \sum T^2$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^3$	$\sum (\frac{5}{2} + \frac{1}{2} \ln T) T^4$	$\frac{1}{2} \sum T^5$	$\frac{1}{2} \sum T^6$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} \sum T^{-3}$	$\frac{1}{2} T_0^{-2}$	$-\frac{1}{2} T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$-\sum T^{-2}$	$\sum T^{-2} \ln T$	$\sum \frac{1}{T}$	$\frac{1}{2} \sum T$	$\frac{1}{2} \sum T^2$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} \sum T^{-3}$	0	0	0	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
$-\frac{1}{2} \sum T^{-2}$	$-\sum T^{-1}$	$\sum \ln T$	$\sum T$	$\frac{1}{2} \sum T^2$	$\frac{1}{2} \sum T^{-1}$	$\frac{1}{2} \sum T^{-2}$	$\frac{1}{2} \sum T^{-3}$	0	0	0	$\sum T^{-2} (\frac{1}{T} - \frac{H_0}{T^2} - \frac{H_0}{T^2} - \frac{1}{2} \frac{H_0}{T^2})$
T_0^{-2}	T_0^{-1}	1	T_0	T_0^2	T_0^3	T_0^{-1}	T_0^{-2}	0	0	0	$\frac{C_p^0}{R} \left \frac{H_0}{T_0} - \frac{H_0}{T_0} \right $
$-T_0^{-2}$	$T_0^{-1} \ln T_0$	1	T_0	T_0^2	T_0^3	T_0^{-1}	T_0^{-2}	0	0	0	$\frac{H_0 - H_0}{R T_0} \left \frac{H_0}{T_0} - \frac{H_0}{T_0} \right $
$-\frac{T_0^{-2}}{2}$	$-\ln T_0$	$\ln T_0$	T_0	T_0^2	T_0^3	T_0^{-1}	T_0^{-2}	0	0	0	$\frac{C_p^0}{R} \left \frac{H_0}{T_0} - \frac{H_0}{T_0} \right $

Figure 1. - Simultaneous least-squares fitting of heat capacity, enthalpy, and entropy.

$$\text{Heat capacity: } \frac{C_p^0}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4.$$

$$\text{Enthalpy } \frac{H_T^0}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln T + a_3 + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{b_1}{T}.$$

$$\text{Entropy: } \frac{S_T^0}{R} = -a_1 \frac{T^{-2}}{2} - a_2 T^{-1} + a_3 \ln T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + b_2.$$

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